1987

The modeling and control of low relative volatility splitters

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The Modeling and Control of Low Relative Volatility Splitters

A thesis written in partial fulfillment
of the requirements for the degree of
Master of Science in Chemical Engineering,
Lehigh University,
Bethlehem, Pennsylvania

by Mark Vincent Finco
January 1987

Distillation columns which separate close boiling components have dynamics dominated by large lags and dead times. A propene/propane splitter at Sun Refining and Marketing, Marcus Hook, Pennsylvania was used as a specific example to investigate the modeling and control of these systems. Data from the splitter was used to build accurate steady state and dynamic models.

Steady state investigations looked at the sensitivity of the column to different disturbances, and yielded steady state gains for preliminary controller analysis via the relative gain. Rating studies quantified the economic incentive for tighter control minimally at $150,000 per year.

Simulation studies on the dynamic model showed unacceptable performance from classical material and energy balance composition control structures, as well as an EVaCS multivariable controller. By far, the best performing composition control structure controlled overhead composition with distillate flow and bottom composition with bottoms flow (D/B structure). This structure is very unconventional, but it's performance was superior to all of the classical structures. The D/B structure was tested over a wide range of regular and irregular operating conditions and performed well. Additional investigations have determined that results from the specific study of propene/propane splitters should be applicable to a range of low relative volatility separations where the dynamic responses are very slow.

First and foremost I would like to thank my parents for their love, care, and concern for me and how I was brought up. Genetics may be 10% of a person's character, but without a doubt, the other 90% comes from the person's environment. I guess I was lucky and got the benefit of all 100%! My parents, as well as all of my family (that includes you, John), have made my stay at Lehigh easier and more enjoyable. I thank you.

If I were to thank everyone who has been instrumental in my professional growth it would take several pages. So, for the sake of brevity, I thank all of the fine students and teachers which I was blessed with through high school. For his motivation and inspiration at Purdue I would like to thank Dr. L. B. Koppel. Thank you Dr. Georgakis for your initial and continued concern for my graduate education. Everything you have done on my behalf is sincerely appreciated. My thanks to my advisor Dr. William L. Luyben. Truely an engineer's engineer (and a farmer's farmer!), you have helped me to keep my feet on the ground and taught me more through your fine example than I would ever be able to thank you for. And finally to Dick Polleck and Arve Holt at Sun Refining and Marketing, for their time and patience while trying to teach me the ways of the 'real world'.

Many thanks to Air Products and Chemicals and the Chemical Process Modeling and Control Center for their financial support over the last two and one-half years. You made it all possible.

A special debt of gratitude goes to all of the people in the Chemical Engineering offices without whom the place would fall apart!

So, thank you Pat, Sharon, Barbara, Monica, Sharon, Gina, Carol, Kay and Mary for all that you have done. Also thank you to my several proof readers, without whom the rough draft of this thesis would have been much . . . rougher; thank you mom, dad, and Susan Kavy.

Finally, thanks to all of my friends at Lehigh and elsewhere. We have gone through all the hard times and fun times together. May there be fewer of the former and more of the latter! To my special friends at school Dave W. (who will never be able to jump), Jeff F. (who will never be a better hunter than his dogs), Joe H. (who just may be a Chemical Engineer and not a Biologist), Don B., Helen B. (or M.), Steven B.(not always a lot of help, but always a lot of fun!), Antoine F. (first of the French connection), Thomas R. (don't ever loose the fine English which I taught you), Don C., Cheri S., Carmen D., Paula D., John D., Apostolos G. (without whom I would have never gotten through State Space Control!), Kannan M., Chris L., Cristian M. (Carla and child), Alain G., Maurizio N., Ding, C.C., Yasu, T.P., Young Soon, Vassilios, Heleni, and all of those who I have forgotten (but I am sure I will hear from soon) thank you and good luck to you all.

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1.0 Introduction

Low relative volatility splitters are dynamic systems dominated by large lags and dead times. Some common characteristics of these columns are:

- large total number of trays (typically 90-200 because of the difficult separation)
- binary mixtures (these separations are at the end of a process where easier separations have already been made)
- high reflux ratios (between 8 - 16 because of the difficult separation being made)
- low column temperature gradient (separation is between close boiling components)
- two tower design (the large number of trays often prohibits building a single tower column)
- discrete composition analysis (usually gas chromatograph)

These properties distinguish the splitters from conventional distillation columns, and make their controllability worthy of special consideration.

There are several chemical systems which fit into the class of 'low relative volatility'. Most notable of these are ethylene/ethane, propene/propane, isobutane/n-butane, and ethylbenzene/styrene. In conjunction with the Process Modeling and Control Center (PMCC) and Sun Refining and Marketing (SUN) a propene/propane splitter (C3 splitter) was studied. This produced an opportunity to study a working process instead of a contrived model with few references to reality, letting us gain the perspective of the engineers who work with the column daily. Studying the specific example of the C3 splitter control might have, however, left the general question of low relative volatility column control unanswered. This concern is addressed and, hopefully, dispelled in section 5. Overall, the benefits of the specific study far outweigh the possible drawbacks, and so, with few exceptions, the balance of this report will concern itself with the specific problem of C3 splitter control.

A four step method was used to approach this problem. It consisted of (1) steady state design, (2) steady state rating, (3) dynamic modeling, and (4) control structure evaluation. The steady state design step compared column designs made on the computer to time averaged plant data for the C3 splitter. The steady state rating ran the computer model through different operating conditions to see how the column performed. This work quantified the economic advantages of tighter control. The dynamic modeling step produced a dynamic computer simulation of the C3 splitter at SUN, and the control evaluation step used this model to test the behavior of different control structures for the C3 splitter.

2.0 Steady State Design

In the previously outlined procedure the degree of detail with which you look at the problem increases with each step. The first, and most basic step, is steady state design. The objectives of the design phase were to gain confidence in the initial modeling assumptions and to develop a vapor/liquid equilibrium correlation which accurately represented the propene/propane system. Results from this phase served as a starting point for the steady state rating step.

2.1 Steady State Plant Data

Time averaged data from the C3 splitter at SUN was assumed to be an accurate representation of the steady state operation of the column. Because column operating pressure cycles from winter to summer, and even night to day, data at three operating pressures was chosen to span the range of possible operating conditions. The resultant range of pressures spanned from 195 to 250 psia (Table 1).

Column Pressure (psia)	195	211	250
Overhead Comp. (mol%)	99.64	99.60	99.60
Bottom Comp. (mol%)	3.8	3.2	11.7
Feed Rate (bbl/hr)	215	231	210
Distillate Rate (bbl/hr)	154	162	150
Bottoms Rate (bbl/hr)	62	66	63
Reflux Ratio	12.53	12.78	14.33
Steam Rate (Mlb/hr)	62.9	66.2	61.6

Table 1: Time Averaged Plant Data

2.2 Mass Balances

To check the accuracy of the plant data, mass and energy balances were made. Mass balances were checked by back-calculating the feed flow rate given the overhead and bottoms flow rates and compositions (Table 2). The mass balances closed tightly, suggesting the external flow and composition data could be relied upon.

Column Pressure (psia)	195	211	250
Measured Feed (bbl/hr)	215	231	210
Back-Calculated:			
Feed (bbl/hr)	201	228	213
Feed Comp. (mol%)	71.6	73.1	74.8
Percent Deviation	6.7%	1.3%	1.4%

Table 2: Mass Balance Results

2.3 Energy Balances

The energy balance was checked by calculating the condenser duty (Qc) in two ways and then comparing the values. The first value was derived by using an energy balance envelope around the entire column. The second value was obtained using an envelope only around the condenser (Figure 1).

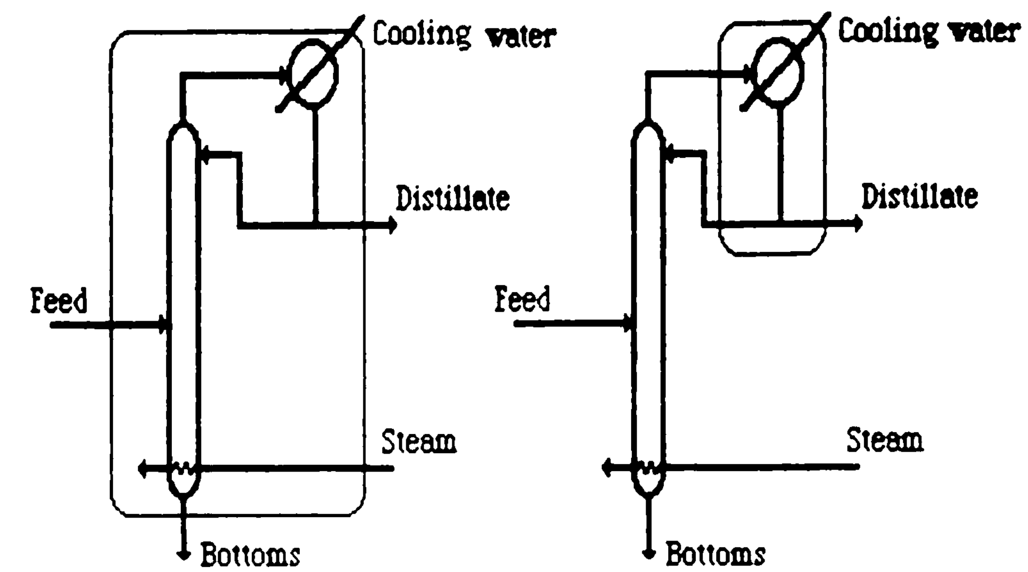


Figure 1: Energy Balance Envelopes

The difference between the two values for Qc represents either the amount of heat which is lost between the reboiler and condenser, or discrepancies in the reflux and/or steam flowrates (Table 3).

Column Pressure (psia)	195	211	250
Envelope # 1, Qc (MM BTU / hr)	64.5	67.7	61.3
Envelope # 2, Qc (MM BTU / hr)	52.2	54.7	53.0
Difference (MM BTU / hr)	12.3	13.0	8.3

Table 3: Heat Balance Results

The heat balances did not close as nicely as the mass balances did. Some of the discrepancy between the Qc's is expected because of heat losses; however, a deviation of not more than 2% of the reboiler duty was expected (1.5 MM BTU/hr). The additional difference was attributed to inaccurate flow measurements, but without a flow and temperature difference measurement on the condenser cooling water it is impossible to find where the discrepancy lies. For the rest of this study it was assumed that the reflux flow measurement was correct.

2.4 Design Programs

First attempts at steady state designs were made on the steady state simulator ASPEN. For several reasons ASPEN was later relaced by a custom written FORTRAN program. The limitations of ASPEN were:

(1) It used a rigorous model of the column, so modeling assumptions could not be tested.

(2) It was difficult to use custom vapor/liquid equilibrium (VLE) routines.

(3) It was meant to be used in the rating mode, not the design mode.

(4) It was very CPU intensive for a large column.

The FORTRAN design program eliminated all of these problems, and allowed us to look specifically at which modeling assumptions and VLE correlations worked best. Because propene and propane are chemically very similar, the assumption of constant molar overflow was made.

2.5 Vapor / Liquid (VLE) Equilibrium

The VLE correlation needed to incorporate pressure and composition dependence in the relative volatility, as well as be easily calculated (no iterative solution). The correlation which resulted gave relative volatility as a quadratic function of liquid composition, where the coeffiecients of the quadratic were linear functions of pressure (Equation 1 and Figure 2). Original data was produced by A.B. Hill (Exxon Chemical).

$$alpha = A0 - A1(x) - A2(x^2) \tag{1}$$
$$A0 = 1.2855 - 0.000446(P) \tag{2}$$
$$A1 = 0.088008 - 0.0001035(P) \tag{3}$$
$$A2 = 0.052215 - 0.00014607(P) \tag{4}$$

Where alpha = relative volatility
x = liquid composition (mole % propene)
P = pressure (psia)

Figure 2 shows this correlation plotted over the entire range of liquid compositions for three pressures.

2.6 Final Computer Designs

Columns were designed at the three operating pressures selected from the plant data (Table 4).

Column Pressure (psia)	Total Trays	Feed Tray (counted from the bottom)
195	162	42
211	163	42
250	155	36

Table 4 : Computer Designed Columns

The columns designed on the computer are very similar to the actual column for the first two operating pressures and slightly different for the third pressure. This suggests that the constant molar overflow assumption is good and that the trays in the actual column are nearly 100% efficient. The designs were made using the reflux ratio, bottom and overhead compositions from plant data, and the back calculated feed composition at each pressure.

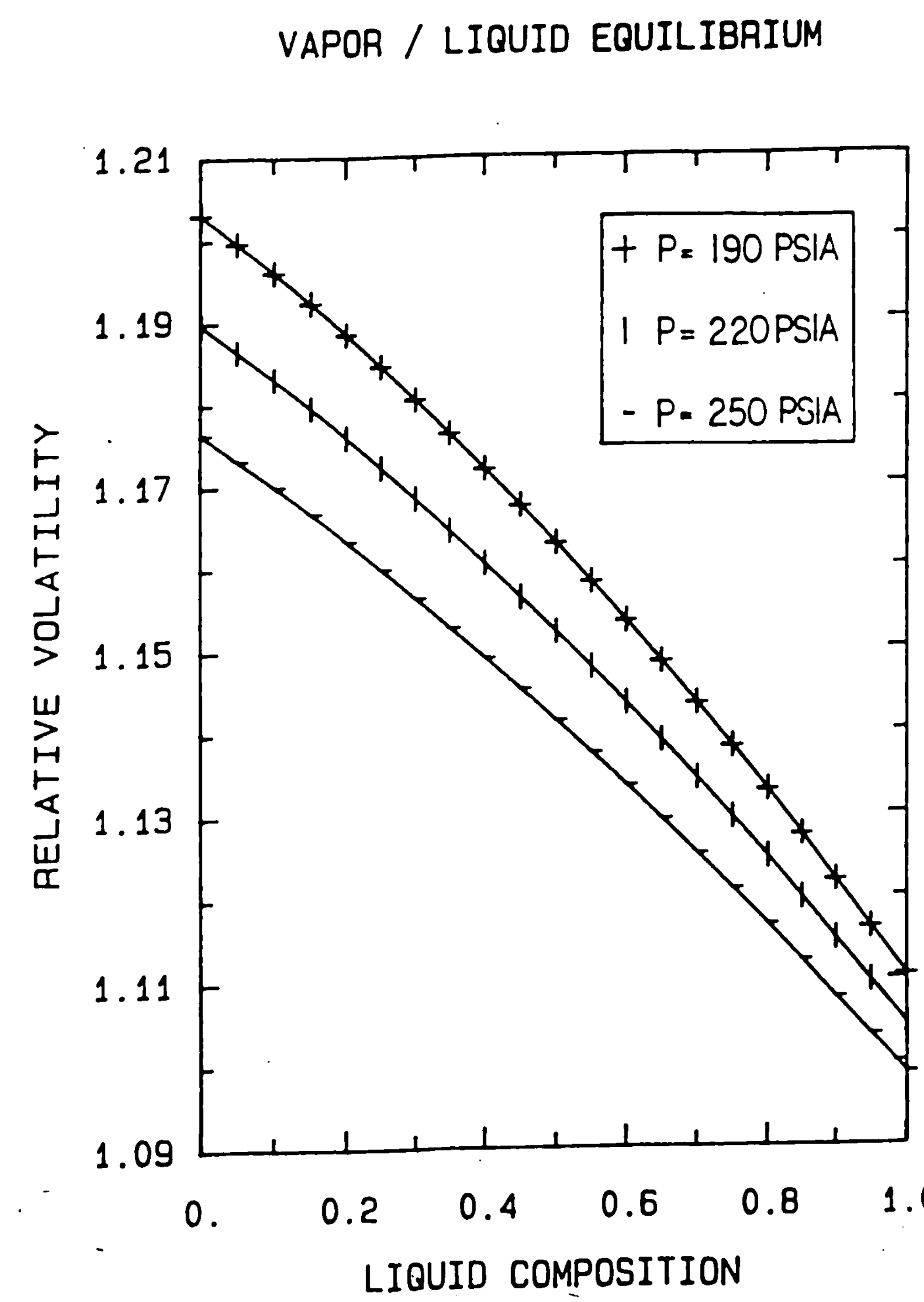


Figure 2: Vapor / Liquid Equilibrium Correlation

3.0 Steady State Rating

Rating tests are performed on an existing piece of equipment (or model thereof) and are meant to show how the equipment performs under various operating conditions. For this study, the rating was performed on the column designed at 211 psia (see section 2.6).

Three types of rating tests were performed with the model. The first rating test found how the column behaved over a range of feed compositions with constant overhead and bottom compositions. Feed composition was varied because it was the unmeasured disturbance most likely to upset the column. The second rating test derived steady state gains, and the third rating test quantified the economic incentive for tighter control. Economic incentive was quantified by calculating the difference between recovered product values and variable operating costs (steam only) for each pair of product specifications.

3.1 Sensitivity

In the following figures the overhead specification is 99.5% propene, and the bottom specification is 2.5% propene. In all cases the feed composition is varied from 60% to 80% propene. The normal operating feed composition is 70%. Figure 3 shows how the internal flows (reflux and boilup) vary to hold product specifications given different feed compositions. The second pair of plots (Figures 4 and 5) show how two other controlled variables, reflux ratio and boilup ratio, vary given the same variation in feed composition. All of the figures show that there is a need for two end composition control.

3.2 Steady State Gains

Steady state gains were obtained by perturbing the column with either reflux or steam. The subsequent variations in overhead and bottom compositions gave the gains between the controlled and the manipulated variables. Units for the gains are mole percent per pound mole per minute.

$$\begin{pmatrix} X_d \\ X_b \end{pmatrix} = \begin{pmatrix} 0.011704 & -0.011283 \\ 0.186370 & -0.186990 \end{pmatrix} \begin{pmatrix} \text{Reflux} \\ \text{Boilup} \end{pmatrix} \tag{5}$$

Because the process is nonlinear, care must be taken to make the perturbation small enough to stay away from the nonlinearities. A 0.07% step was used to derive these gains.

3.3 Economic Incentives

In order to quantitatively demonstrate the need for tighter control, rating tests were performed which showed how recovered product values and variable operating costs change given different product specifications. Moreover, these rating plots show that there are optimum setpoints for the overhead and bottom products. In Figure 6, 'Worth'. (the sum of the product values minus the steam costs) is plotted versus bottom composition for several values of overhead composition. There is a maximum dollar output of the column at x_d=99.5%, and x_b=2.5%. The value that corresponds to the maximum is $5,276 per hour with :

distillate value (>99.5%) = $0.16 / lb.
bottom value (<11%) = $0.11 / lb.
steam value = $5.00 / MM BTU

Compared to current operation (x_d=99.6%, and x_b=6%), simply changing the product specifications could save $19 per hour or approximately $160,000 per year! This saving is a conservative estimate because poorer operating conditions occasionally exist where x_d=99.6%, and x_b=12%. Under these conditions the lost profit is $45 per hour or $1080 per day.

Several interesting observations should be made from Figure 6.

(1) The curves can not be extrapolated to distillate compositions less than 99.5%. This is because below 99.5% the distillate has only fuel value (approx. $0.08/lb) or needs reprocessing. Note that the 99.5% specification is not a hard constraint but is the minimal average composition of the overhead.

(2) Once overhead specifications are met there is more economic incentive to keep bottom composition at setpoint rather than the overhead composition at setpoint (Figure 7).

(3) The optimum bottom specification decreases as the overhead specification increases.

(4) This whole analysis is based on the previously mentioned product and energy values. Given a varying economic climate these figures must be recalculated to find current optimum product specification setpoints.

From this point forward, all investigations will be performed on a column operating at optimum specifications (x_d=99.5%, and x_b=2.5%)

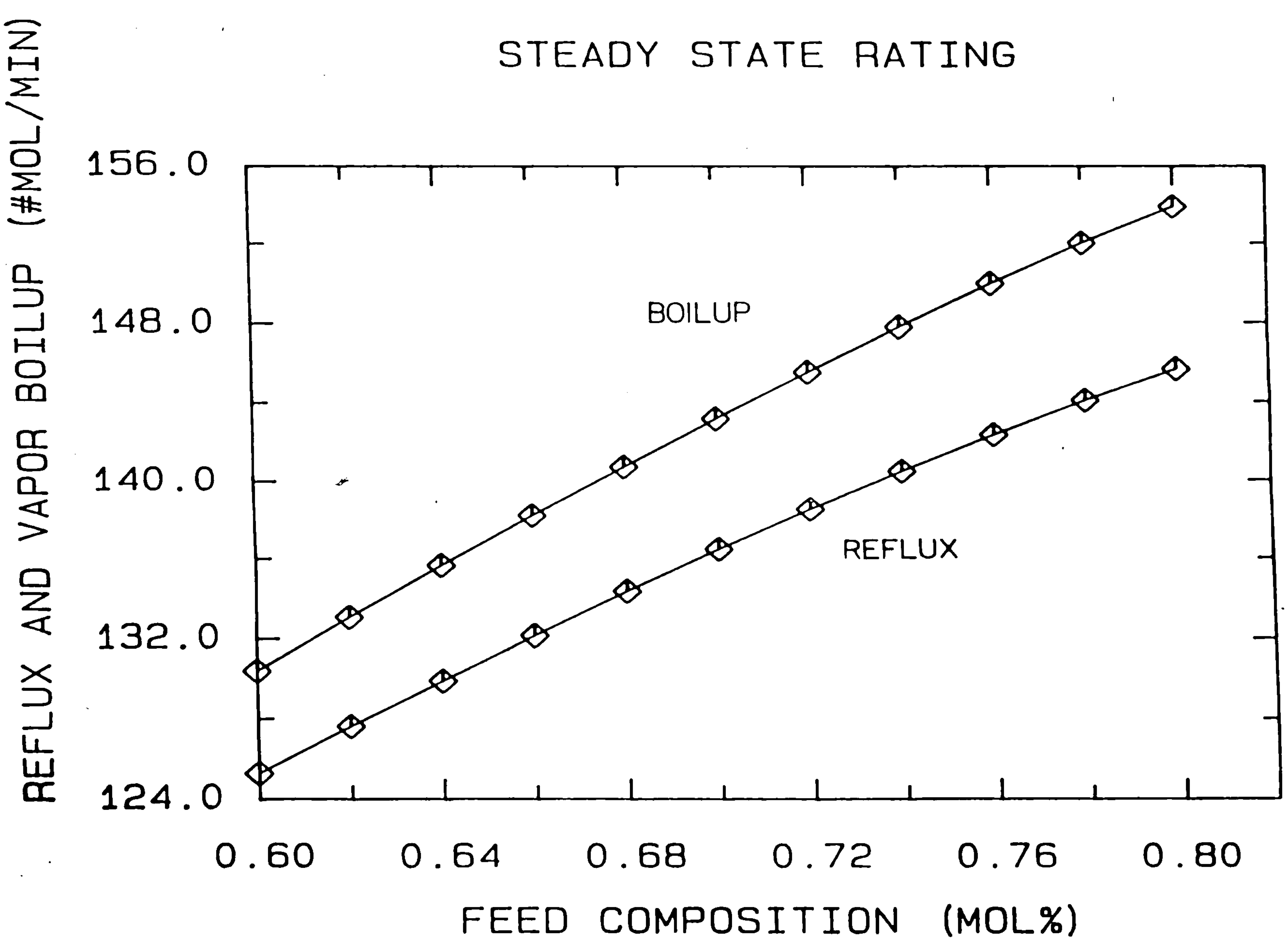


Figure 3: Reflux and Boilup vs. Feed Composition

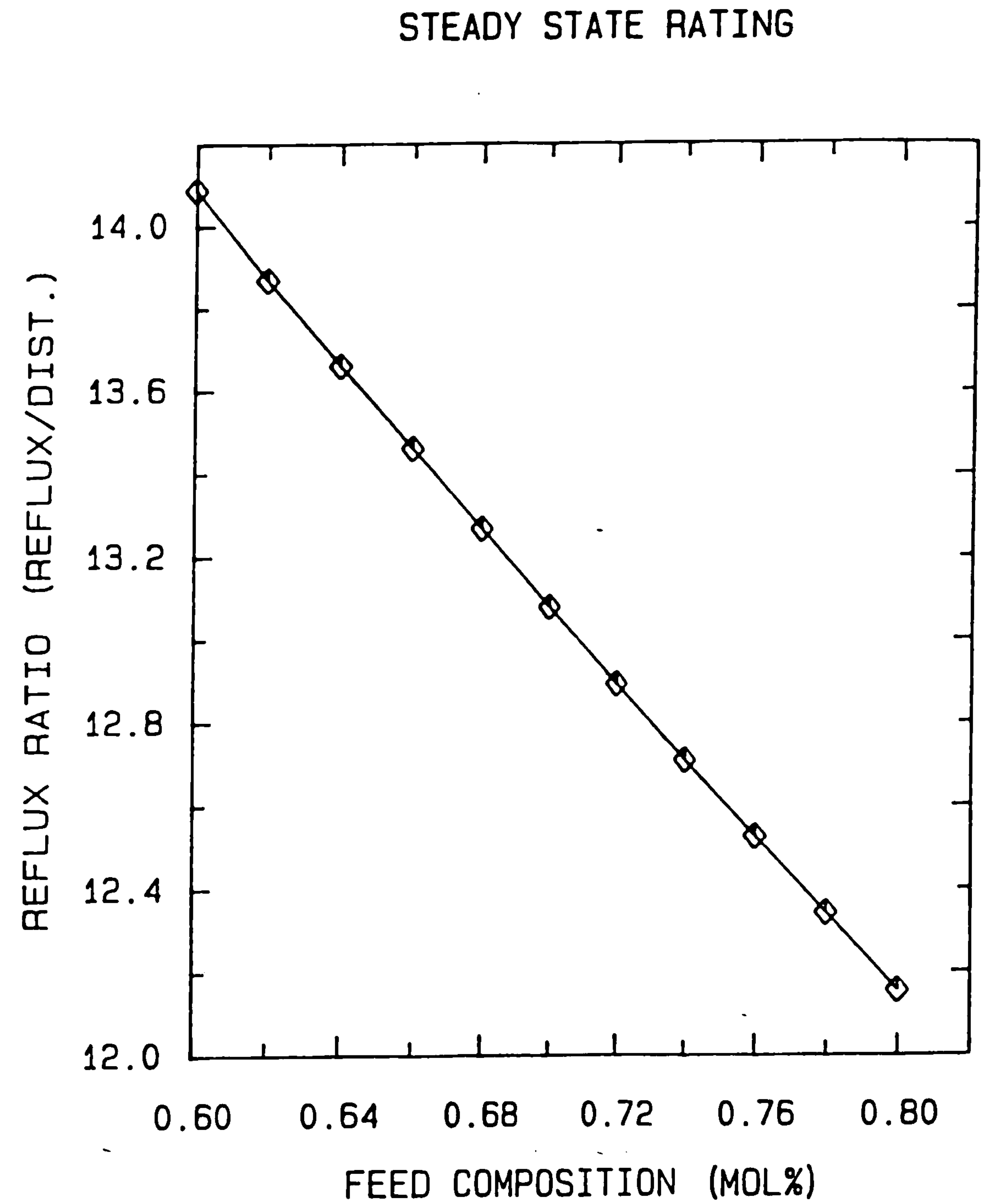


Figure 4: Reflux Ratio vs. Feed Composition

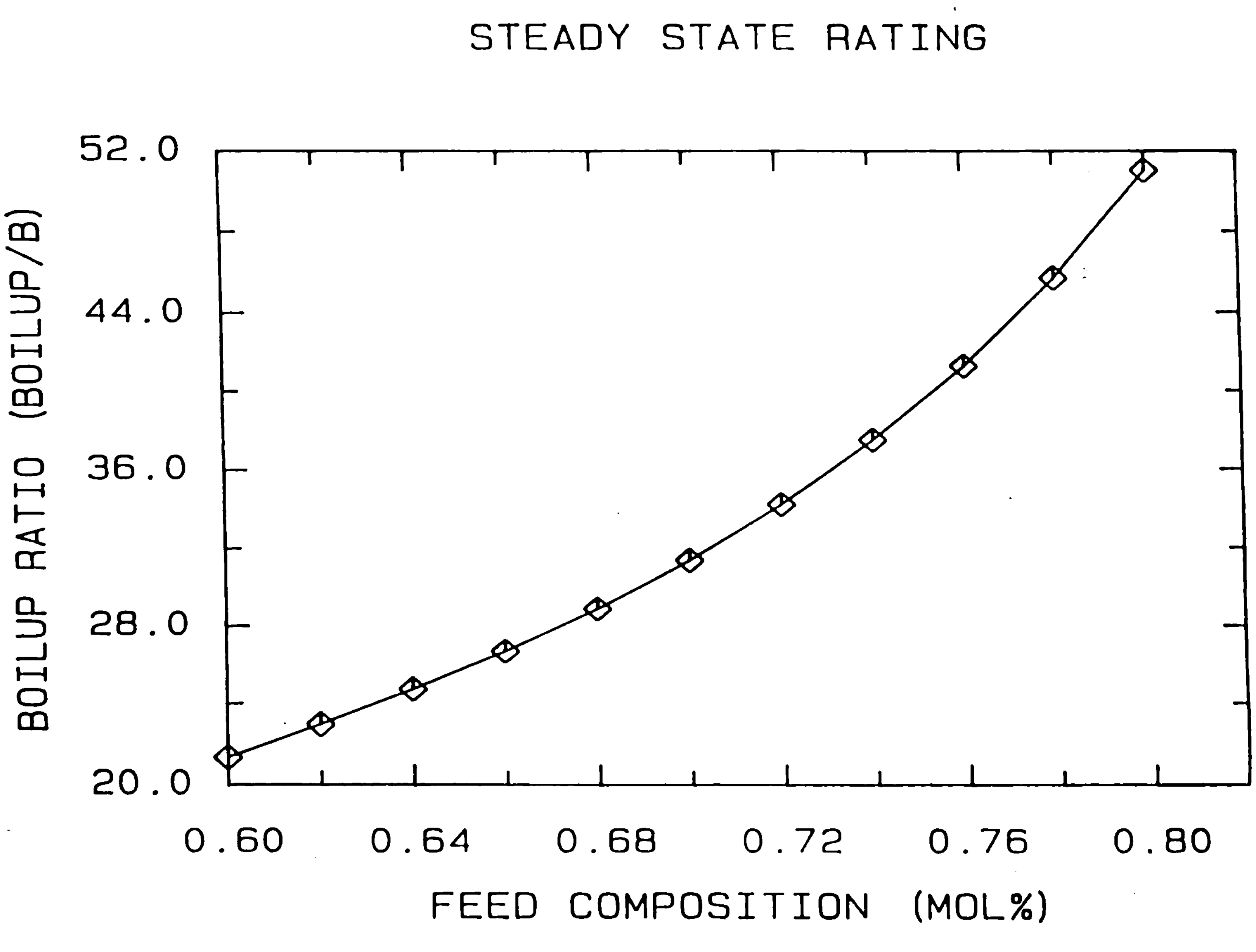


Figure 5: Boilup Ratio vs. Feed Composition

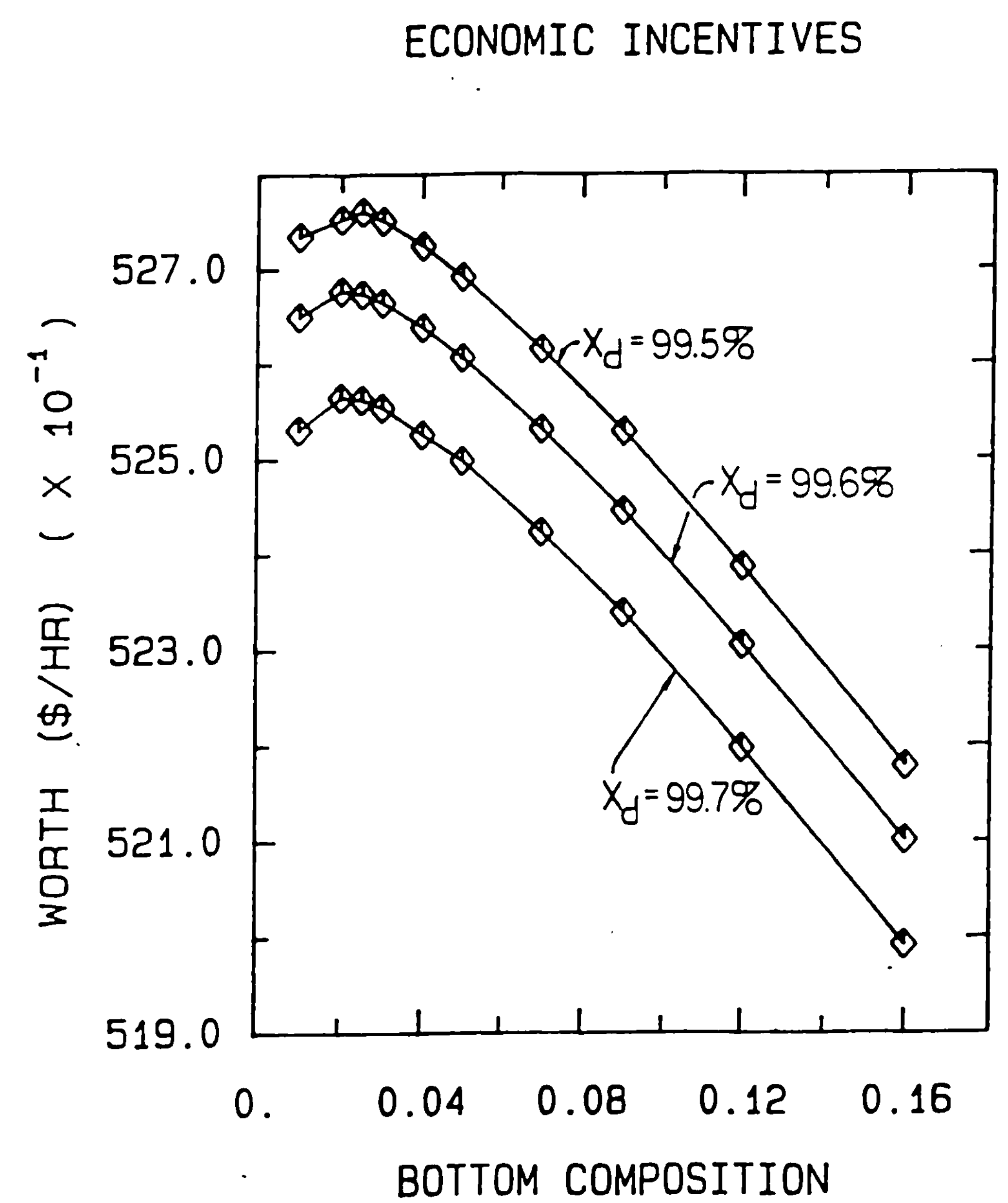


Figure 6: Worth vs. Bottom Composition

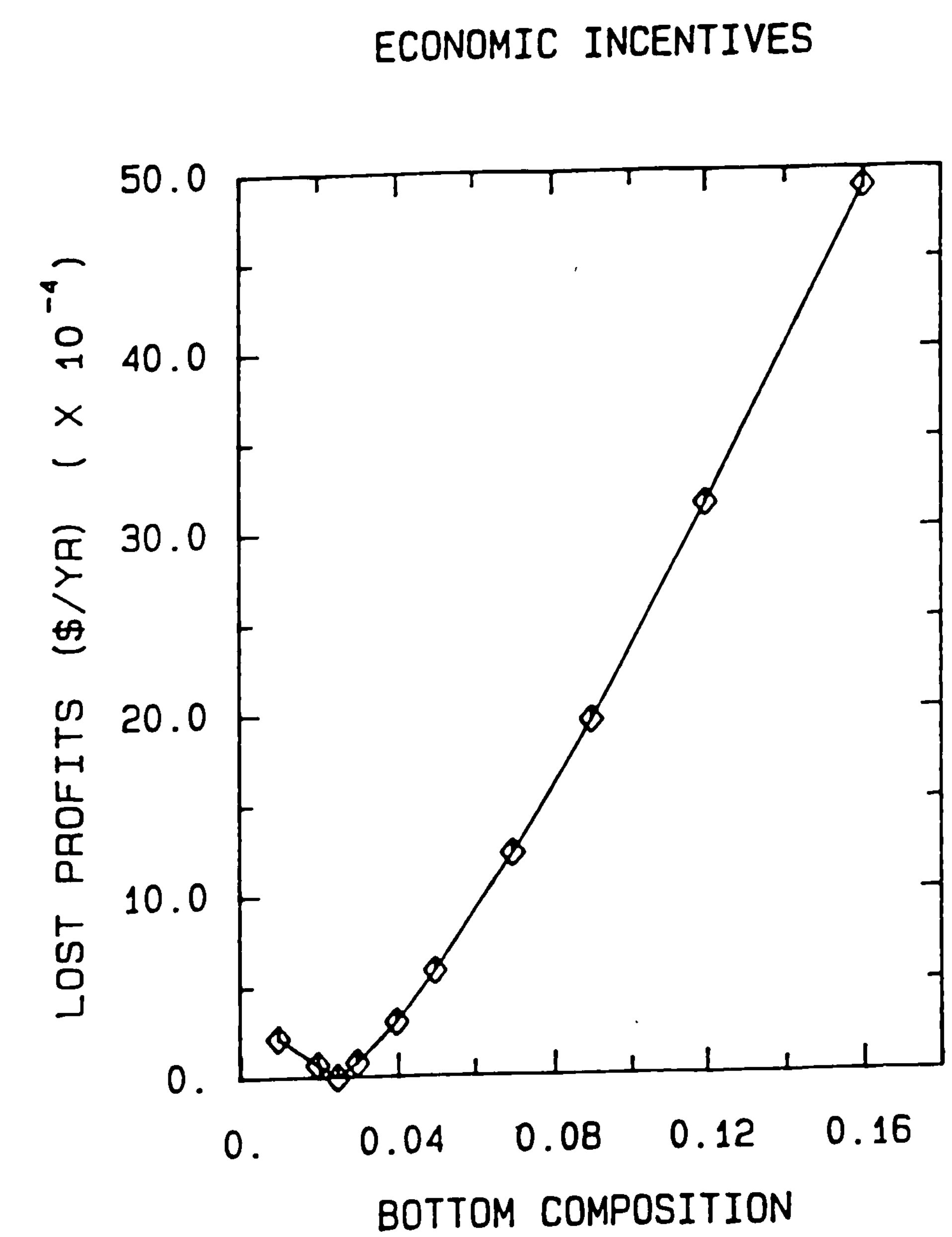


Figure 7: Lost Profits vs. Bottom Composition

4.0 Dynamic Modeling

The initial model of the column had several basic modeling assumptions and details were added to the model when deemed necessary. The initial model assumed (1) constant molar overflow, (2) constant and equal tray holdup, (3) constant and equal tray to tray pressure drop, and (4) perfect level control. Experience from plant pulse tests then added to the detail of the model

4.1 The Actual Column

The specific column being studied is located at Sun Refining and Marketing, Marcus Hook, Pennsylvania. It is one of two C3 splitters which run in parallel in the poly plant at SUN. Normal operation has one of the splitters running at capacity and takes feed swings with the second column. The column in question has 160 trays (18 inch spacing), with feed entering at tray 44 (counted from the bottom). Because of the large number of trays the column is built in two sections. This creates an additional holdup between the two towers of the column. Twin stab-in reboilers are used in the base of the column, and water is used as the cooling medium. The water flows fully open which lets the column pressure cycle as the weather, time of day, or season dictates. Figure 8 is a pictorial summary of the column characteristics.

4.2 The Column Model

There are several key characteristics of the model which need to be explained. The next several sections will address the specific characteristics and assumptions which were used to model the C3 splitter.

4.2.1 Initial Data

Dynamic models require a set of process variables to start the simulation. A rating program was used to adjust the reflux and vapor boilup to get precisely 2.5% in the bottoms and 99.5% in the overheads. After the rating was done, the process flows, composition profile, and pressure profile was used as the lined-out starting point for further simulations.

4.2.2 Feed and Feed Split

Feed to the column is two phase. Because the relative volatility is low and true flash calculations are iterative (ie. computer intensive) the feed split was done using an 'approximate flash'. In the approximate flash the liquid and vapor compositions and the feed composition were assumed equal. This was a fair assumption because the relative volatility was very close to one. Only the liquid and vapor rates varied as feed condition varied. This approximation gave a quickly calculable and accurate approximation of the affects of feed quality on the column.

4.2.3 Liquid Levels

In the two tower design there are three liquid levels to be concerned with. They are the bottom of the lower tower, the bottom of the top tower (sometimes called middle level), and the accumulator level. In each of these cases the span of the level transmitter was 32 inches, and the steady state holdup (or 50% level) was assumed halfway between the level taps. Values for the steady state holdups were found using the blueprints of the column. From the geometry of the vessels, numbers were calculated which converted changes in holdup to changes in the particular level.

Vessel	Holdup (lb-mol)
Accumulator	725.9
Top tower sump	261.9
Bottoms	498.1

Table 5 : Holdups

4.2.4 Differential Equations

Any distillation column may be thought of as a series of connected process units. Among the units are feed trays, regular equilibrium stages, reboilers, accumulators, and sidestream trays. When combined, the differential equations which model these units form a set of coupled differential equations which model the entire column. The set of differential equations describing the C3 splitter was built in this way. Figures 9 and 10 give a pictorial derivation of the different unit equations used.

Details were added to the initial model as dictated by the plant data. The major change to the model was the addition of a second (hydraulic) differential equation per tray. The liquid traffic in the column needed to be delayed in order to give an accurate representation of the column's behavior. First approaches lumped the tray hydraulic lags into several sections and approximated these lumps with pure dead time. This approach was suggested to save computing time. It was found, however, that this method caused the compositions in the middle of the column to behave very unnaturally given a 2% feed composition disturbance (see Figure 11). A possible explanation of this behavior is that lumping the lags into deadtimes creates an artificial accumulation of material in each section while it waits for new liquid flow information to propogate. This behavior occurred regardless of the number of trays in each section, and was eliminated by adding a second differential equation to each tray (Equations 6 and 7 below).

$$L_n = L_{ave} + (M_n - M_{ave}) / Beta \qquad (6)$$

$$dM_n/dt = L_{n+1} - L_n \qquad (7)$$

where, L = liquid flows

M= liquid holdup

Beta= hydraulic constant

Beta was adjusted to give responses and deadtimes similar to the actual column. For this case a value of 0.18 minutes was used.

4.2.5 Sampled and Shifted Data

On line gas chromatographs automatically sample the overhead and bottoms streams every five (5) minutes. Since this project's conception in May 1985, the sampling time has been halved from ten minutes to the current five minutes. The decrease in sampling time has certainly made the closed-loop control of the column much tighter, and has been taken into account for all ensuing control structure evaluations. Because it takes five minutes to process a sample, the signal which is controlled is not only sampled but also delayed by one sampling period (Figure 12). Likewise, the manipulated variables are put through a first-order hold.

4.2.6 Model Responses

The final model was tested with pulse tests of the manipulated variables. The pulse tests for the L/V control structure (L controlling distillate, V controlling bottoms) are shown in Figures 13 and 14. In all of these figures the manipulated variables were pulsed +2% for the period between 50 and 100 minutes (see figures). This structure gives a typical response with relatively quick initial response to the pulse and a long trailing response back to setpoint. These responses suggest column time constants of between 600 and 900 minutes.

The response of the D/V structure (D controlling distillate , V controlling bottoms) in Figures 15 and 16 gives a smooth response to changes in D, but pulses in V show inverse response characteristics. This is caused by the accumulator level control scheme (accumulator level controlled with reflux flow). With this structure, the change in vapor boilup has two effects. For increased vapor, the first effect is to boil more lights out of the bottom and decrease the purity in the overhead. The second effect is to increase the accumulator level which increases the reflux flow. The increased reflux then increases the amount of lights in the bottom and overhead; thus, the inverse response characteristic is produced. Note that the V response of the D/V structure settles out much more quickly than that of the L/V structure.

4.3 Plant Pulse Tests

Pulse tests on the C3 splitter at SUN were performed on April 14-16, 1986 and August 12-13, 1986. Over the course of these days, pulse tests were made with the steam and reflux (L/V structure). It was difficult to make pulses where the response was distinguishable from the background noise without irreversibly upsetting the column. Out of the five days of testing, one reflux and one steam pulse were clean enough to be clearly recognized. The overhead composition proved to be insensitive to changes in either reflux or steam, and therefore was often the limiting observation determining pulse magnitude.

From the pulse test results the Beta parameter was adjusted to match the plant data. This modified model and plant data are compared in Figures 17 and 18. This favorable comparison gave us confidence that the control studies on the model would accurately approximate the response of the actual column.

4.4 Identification

In preparation for control studies transfer function models were needed. It would be advantagous to derive transfer function models directly from the plant data, but there are problems doing this with systems which have very large time constants. The primary reason is that either Fourier transform or time series analysis needs at least one or two time constants of data for the analysis to yield plausible results. In systems such as these, with time constants of 12 - 15 hours, this is not possible at the plant. For this reason all identification was done with responses of the model and not with the actual plant data.

An alternative method to overcome this problem was proposed. The method is known as the 'dual pulse' method and uses a negative and a subsequent positive pulse instead of the usual single pulse to identify the process. Clearly, the advantage of this is that the dual pulse response wanes 6 - 8 times more quickly than the single pulse response, and therefore this method is attractive for systems with large time constants.

Both methods have been used to identify the column model. The identification was performed using frequency response techniques. Table 6 shows the results from each pulsing method on the column model for perturbation magnitudes of 0.5%.

The steady state gains derived from the pulse tests are not exactly those found with the steady state rating program. The nonlinearity of the model causes this and is why gains from the rating (where perturbations were .07%) were used in the RGA analysis. Note when comparing rating gains and gains derived from the pulse tests that the units are different and must be changed to make a comparison.

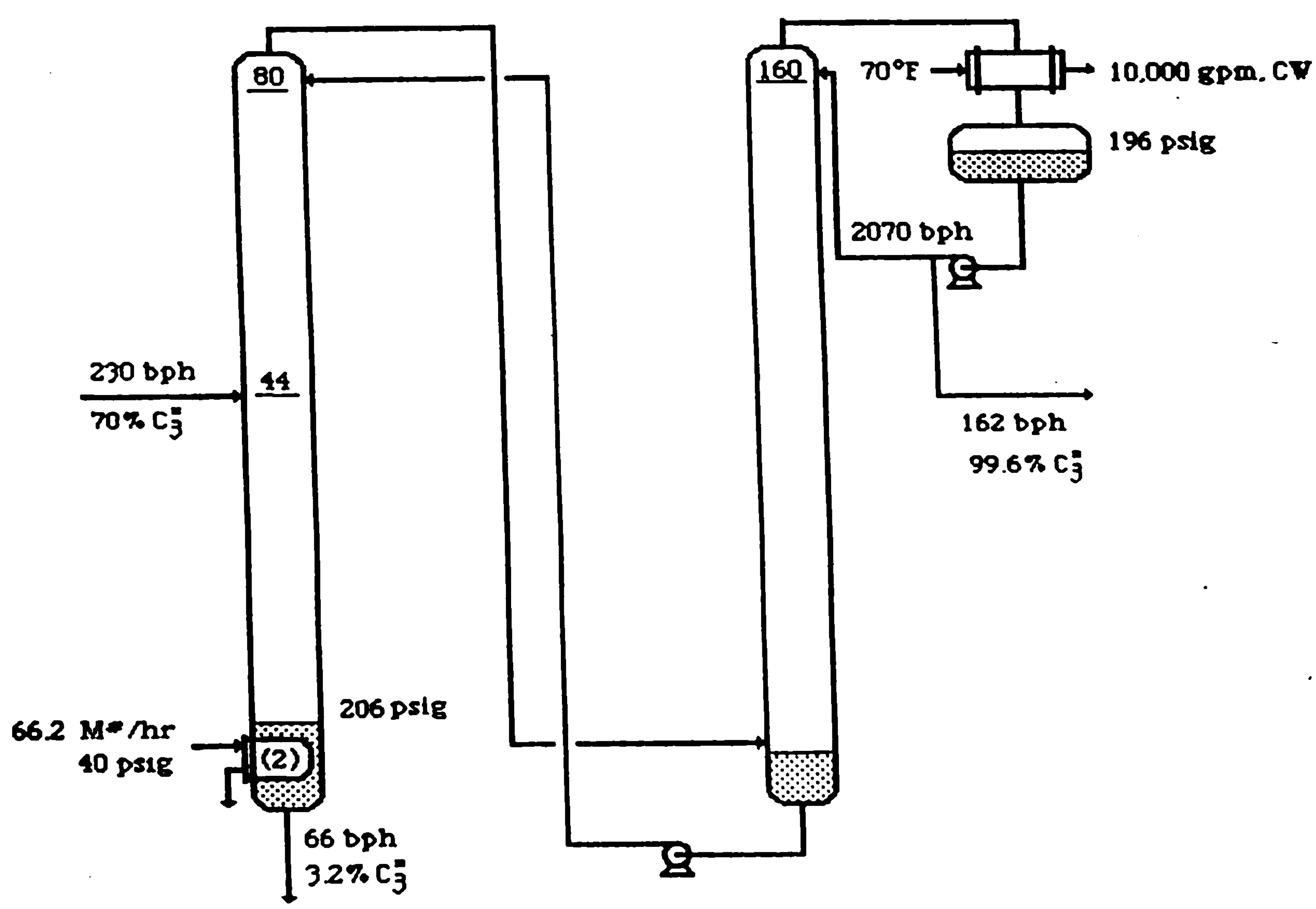
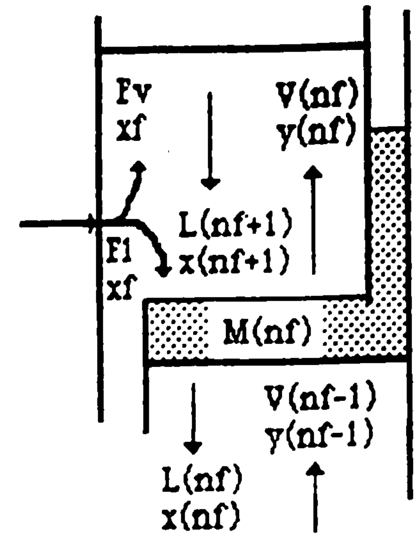


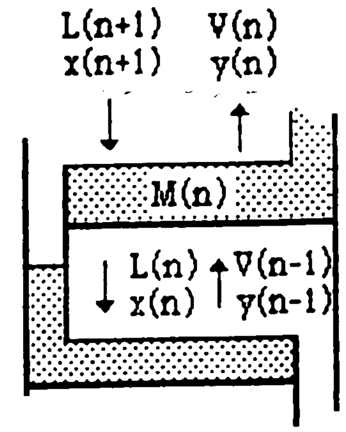
Figure 8: T-10 Splitter at SUN



Feed Tray

$$\frac{d}{dt}[M(nf) * x(nf)] =$$

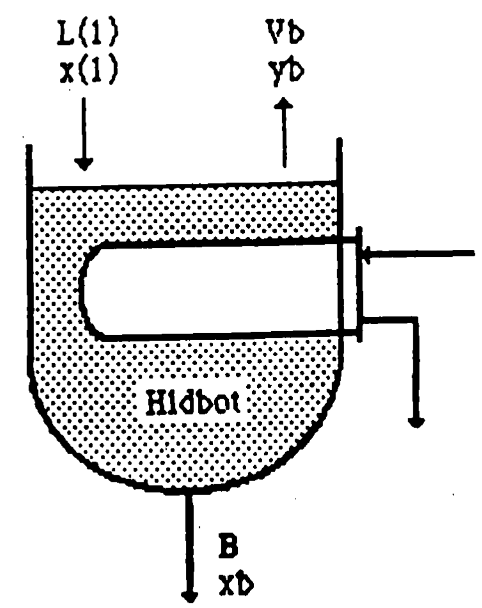
$$Fl * xf + L(nf+1) * x(nf+1) + V(nf-1) * y(nf-1) - L(nf) * x(nf) - V(nf) * y(nf)$$



Normal Tray

$$\frac{d}{dt}[M(n) * x(n)] =$$

$$L(n+1) * x(n+1) + V(n-1) * y(n-1) - L(n) * x(n) - V(n) * y(n)$$

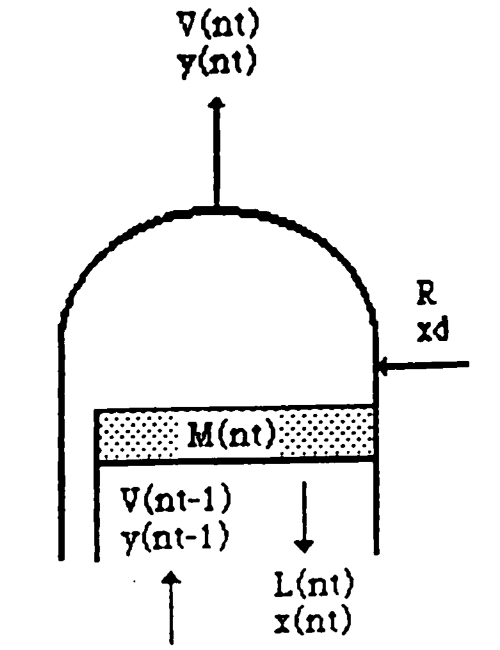


Bottoms

$$\frac{d}{dt}(Hldbot * xb) =$$

$$Vb*yb - L(1)*x(1) - B*xb$$

Figure 9: Derivation of Differential Equations (Bottom)

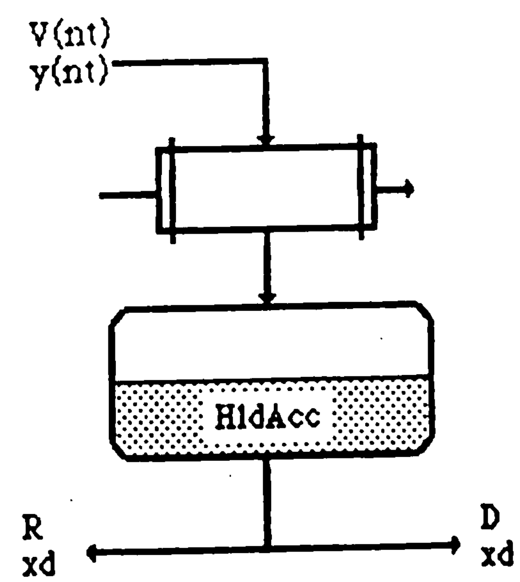


Top Tray

$$\frac{d}{dt}[M(nt) * x(nt)] =$$

$$V(nt-1) * y(nt-1) + R * xd$$

$$- V(nt) * y(nt) - L(nt) * x(nt)$$



Accumulator

$$\frac{d}{dt}(HldAcc * xd) =$$

$$V(nt) * y(nt) - (R + D) * xd$$

Figure 10: Derivation of Differential Equations (Overhead)

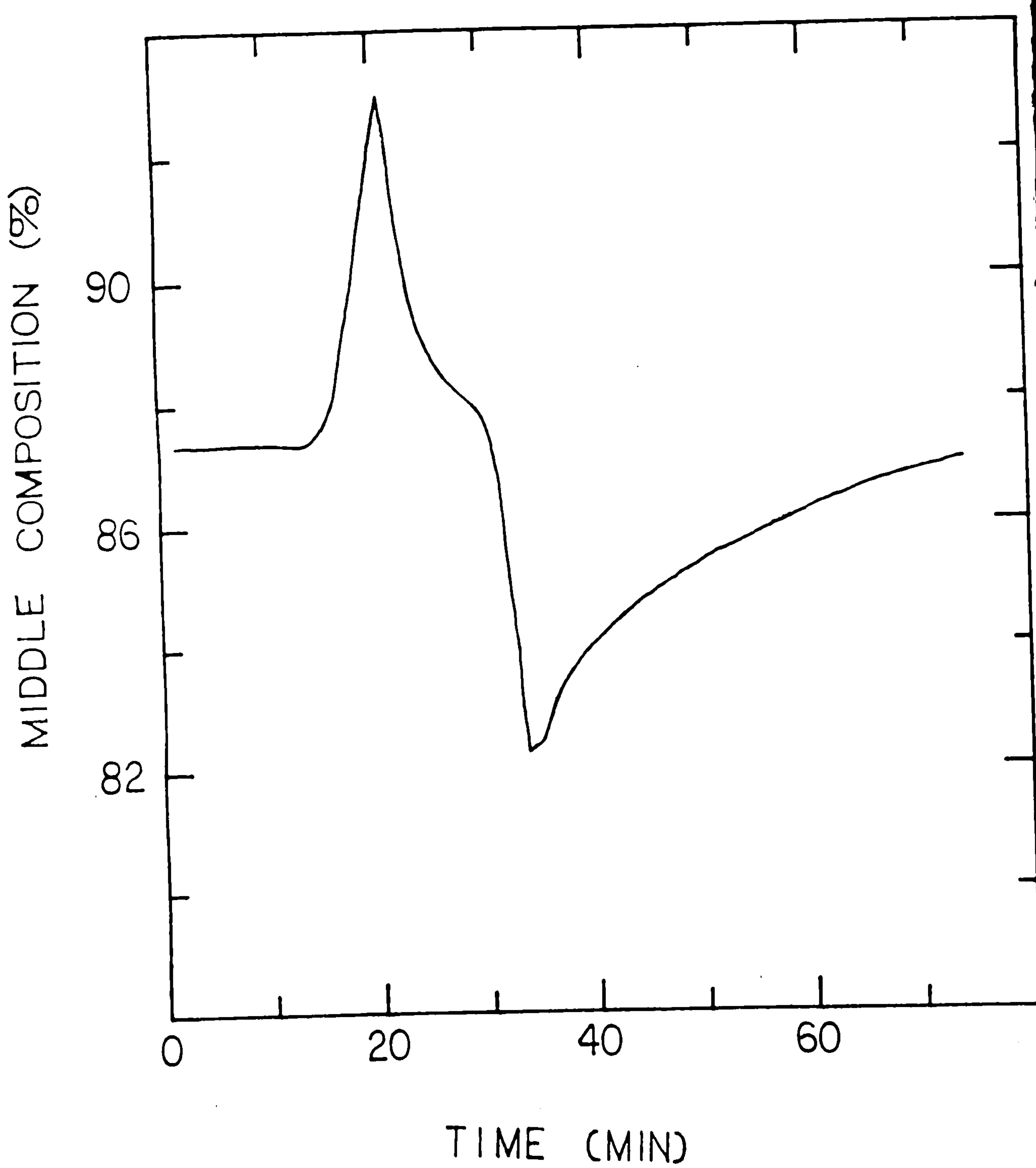


Figure 11: Lumped Hydraulics Column Response

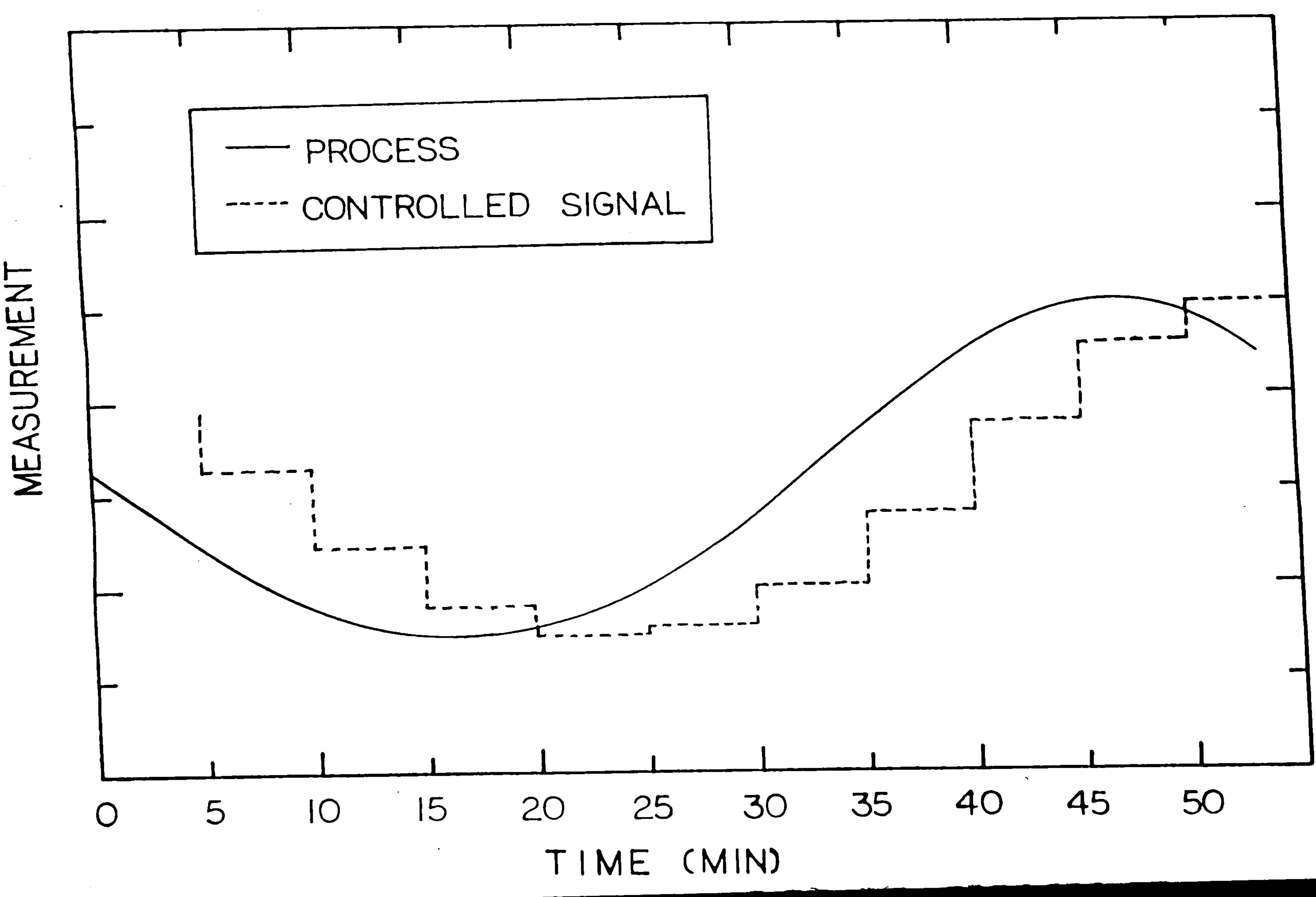


Figure 12: Sampled and Shifted Effects

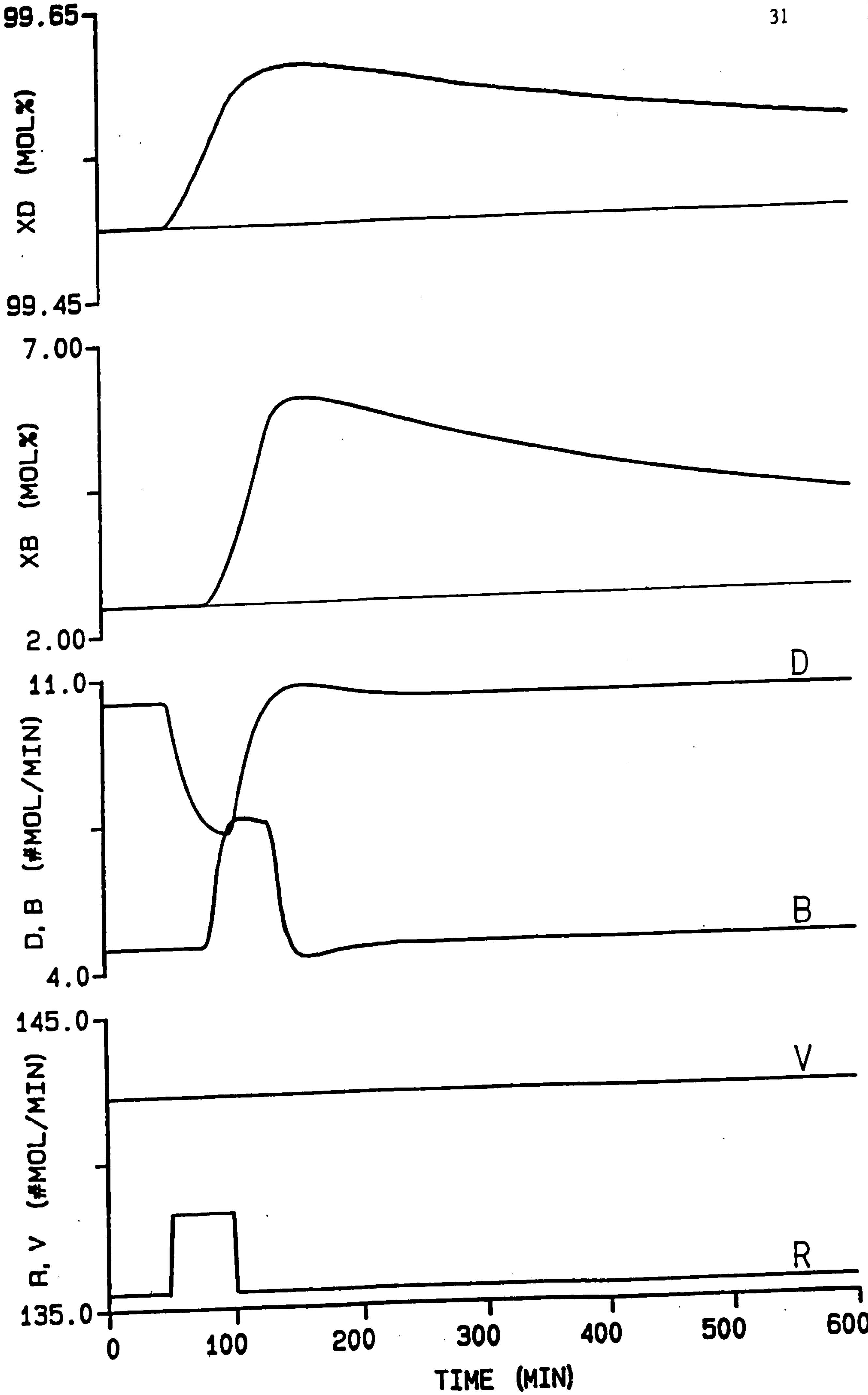


Figure 13: Open Loop Response of L/V Structure, L pulsed

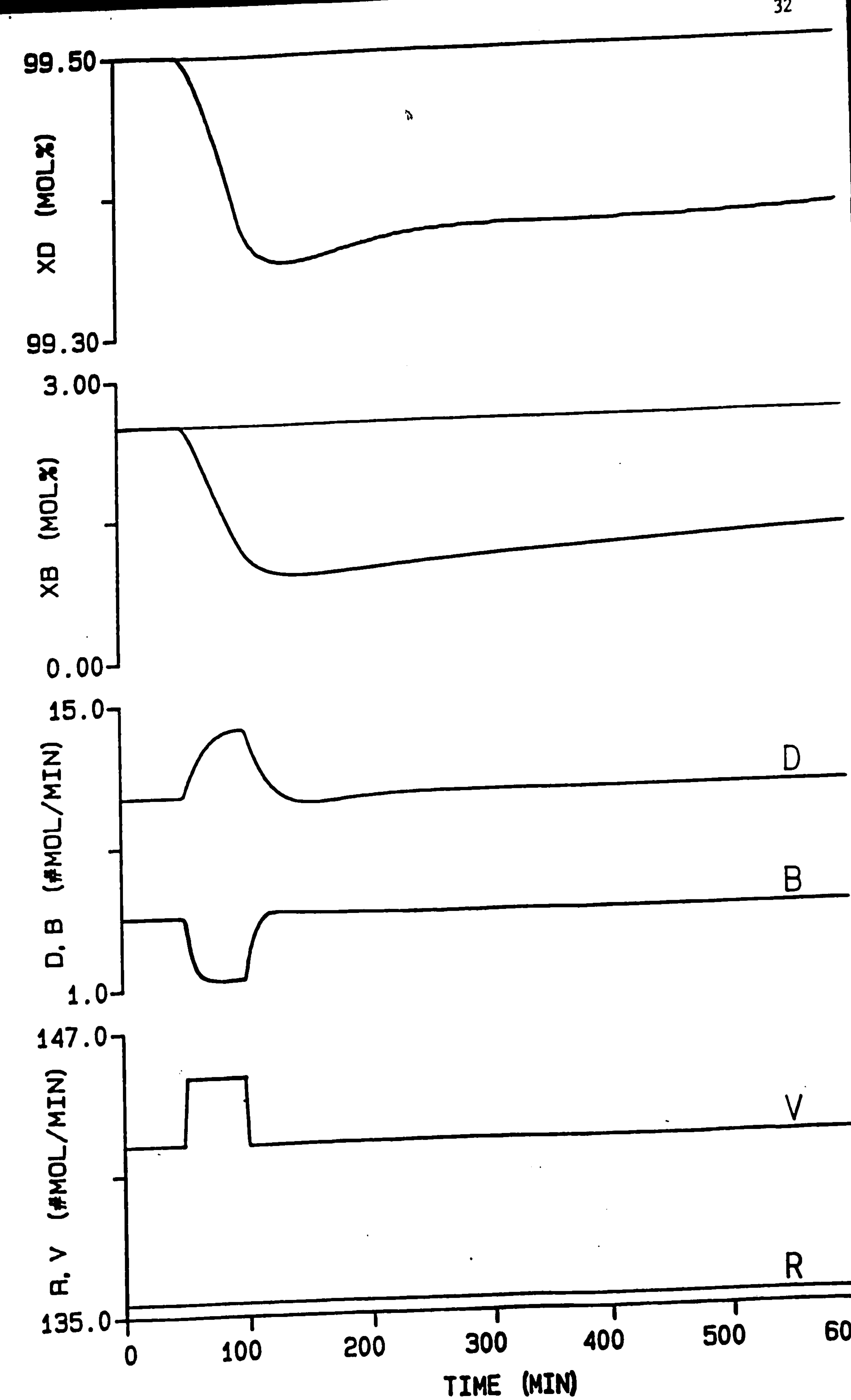


Figure 14: Open Loop Response of L/V Structure, V pulsed

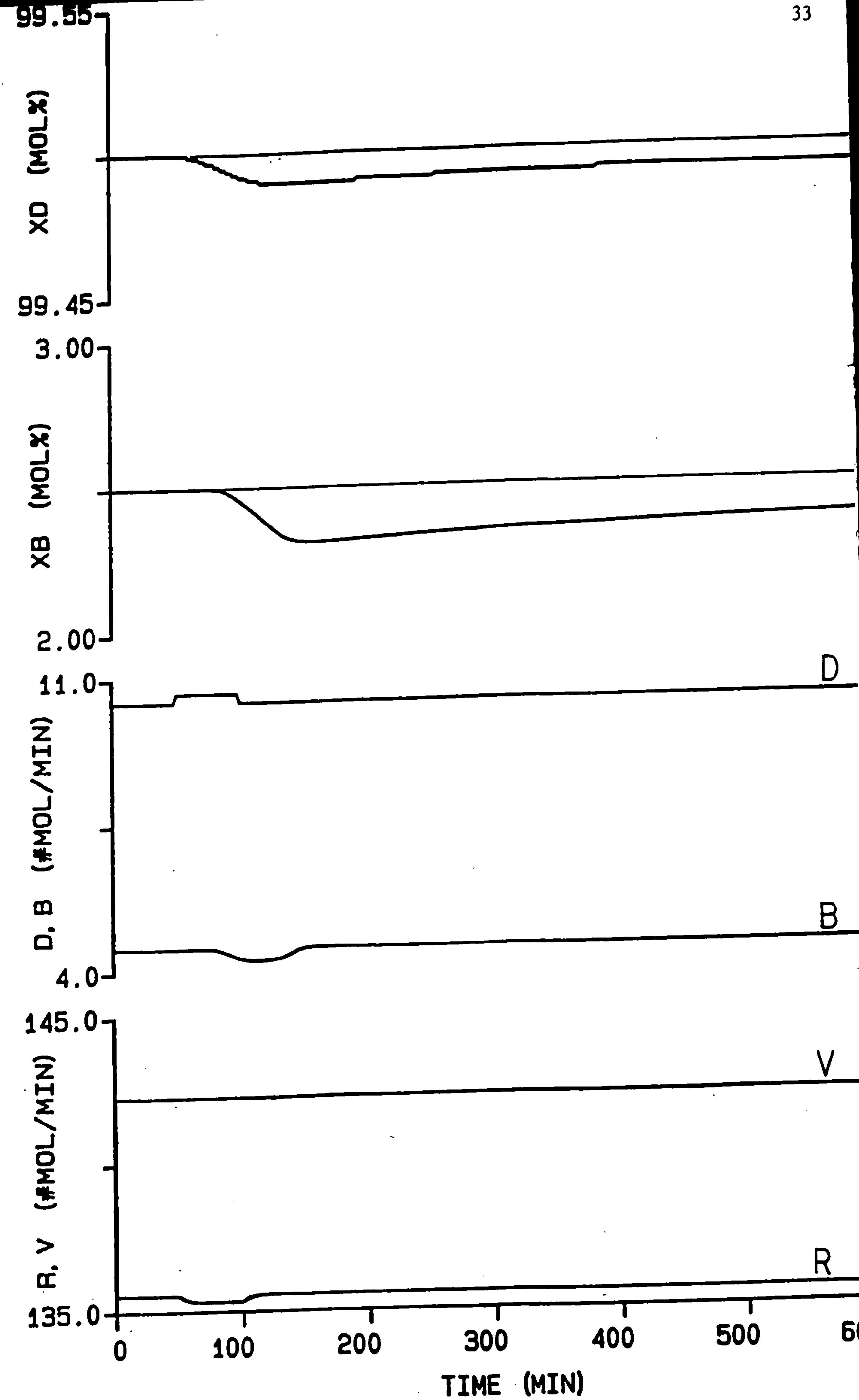


Figure 15: Open Loop Response of D/V Structure, D pulsed

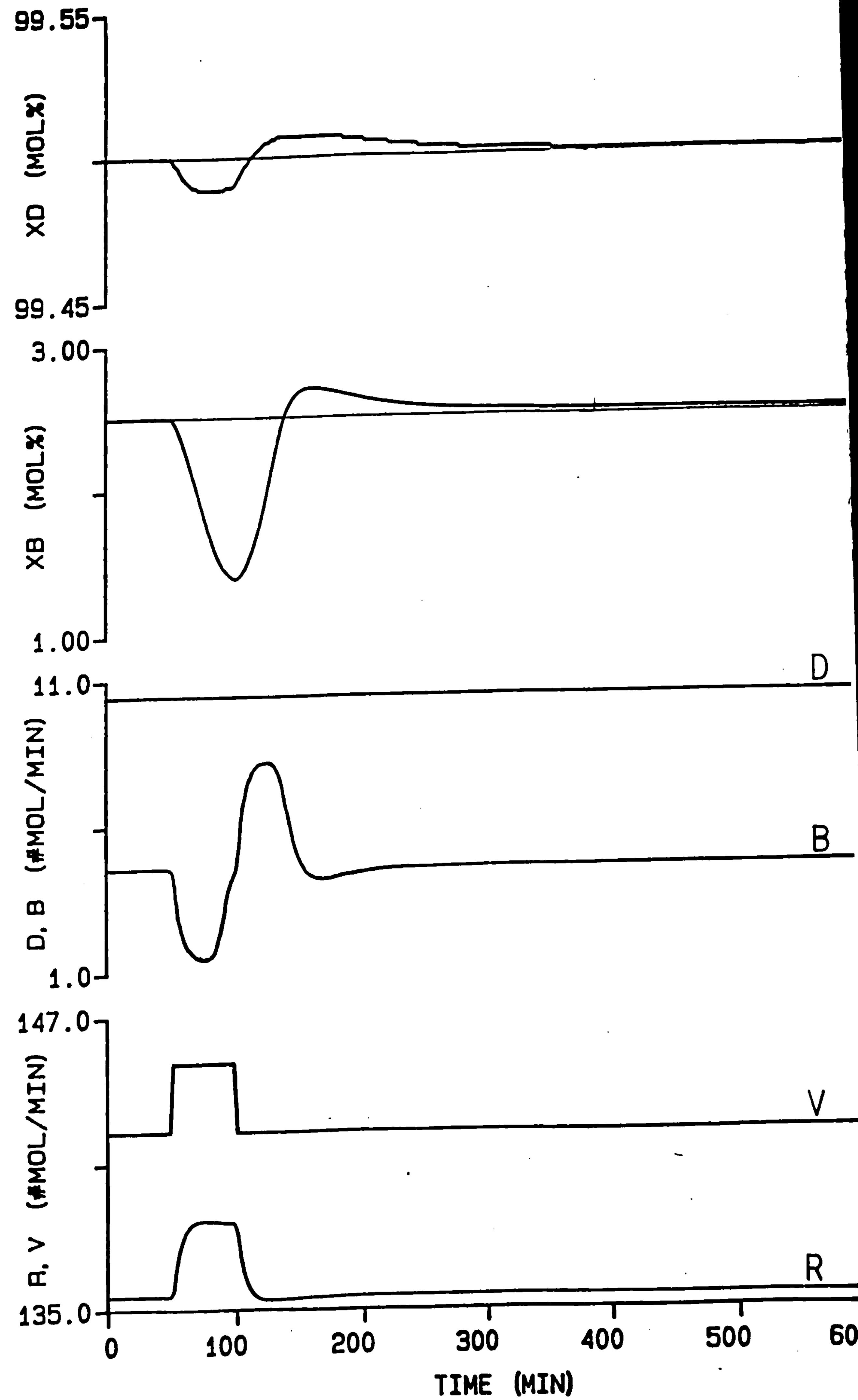


Figure 16: Open Loop Response of D/V Structure, V pulsed

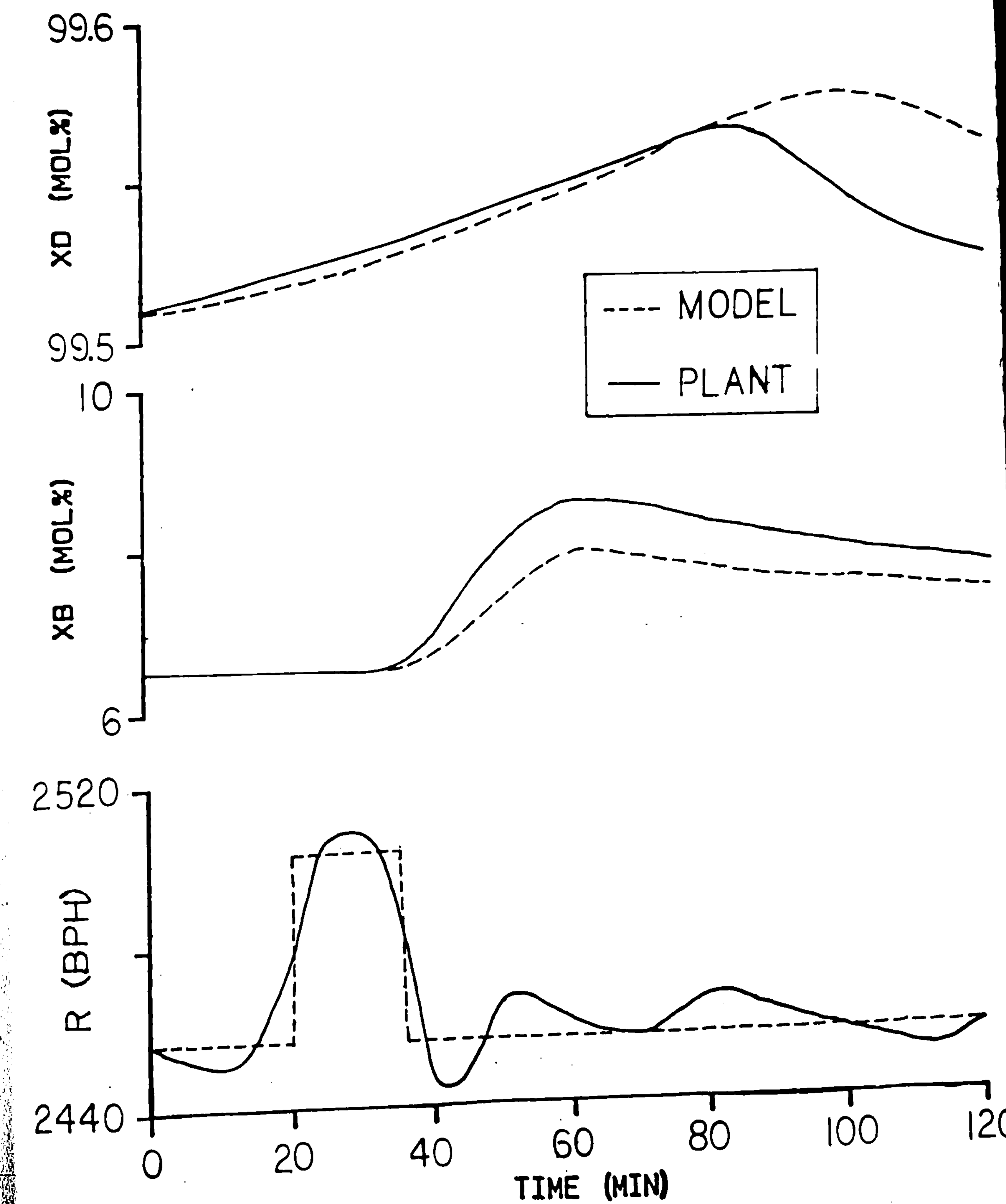


Figure 17: Plant Pulse Test Compared to Model, L pulsed

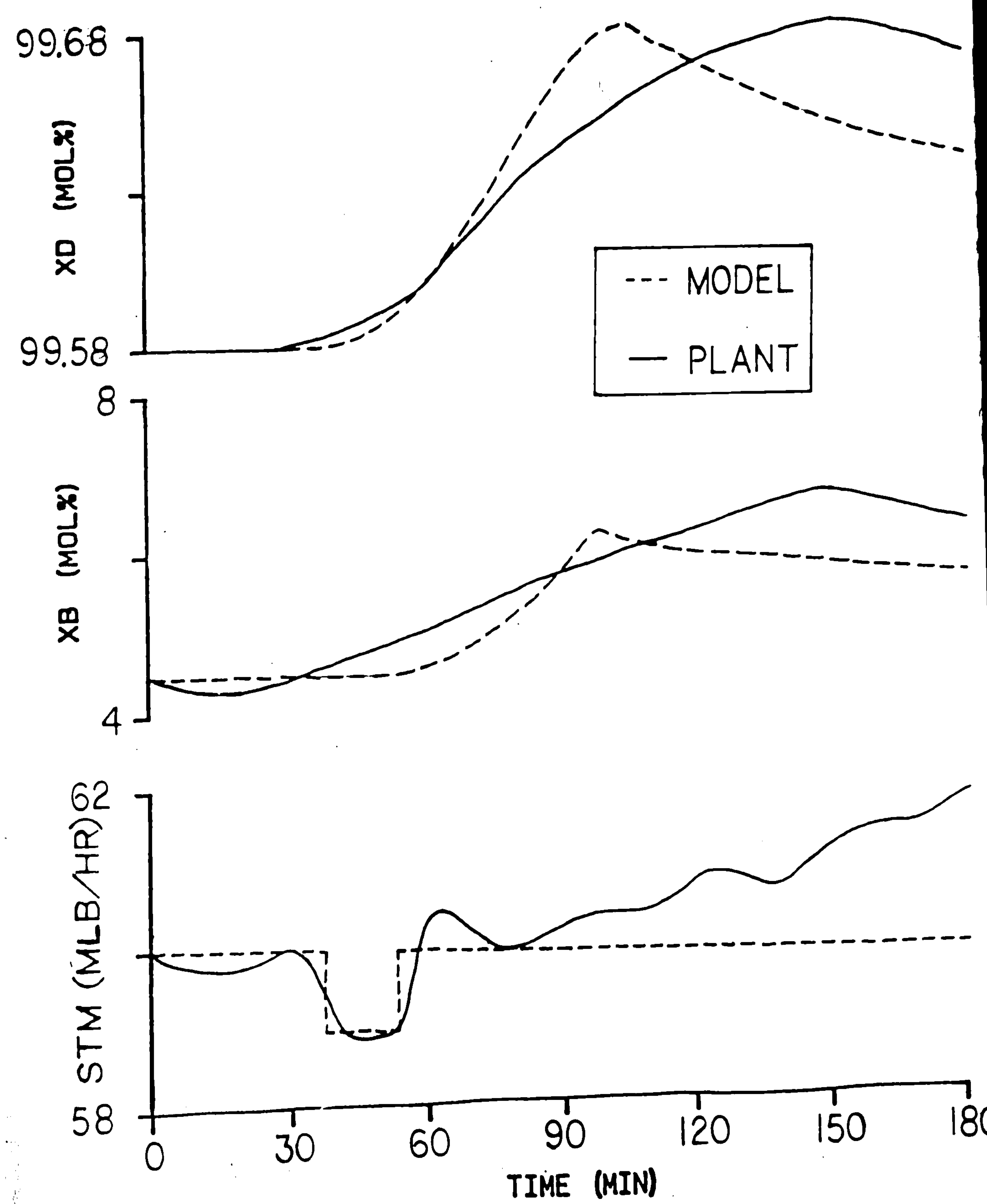


Figure 18: Plant Pulse Test Compared to Model, V pulsed

$$\begin{pmatrix} X_d \\ X_b \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \begin{pmatrix} \text{Reflux (lb-mol/min)} \\ \text{Steam (lb/min)} \end{pmatrix}$$

	Single Pulse	Dual Pulse
g_{11}	$\frac{(0.00854)\,e^{-3s}}{(951s+1)(18s+1)}$	$\frac{(0.00504)\,e^{-3s}}{(612s+1)(10s+1)}$
g_{12}	$\frac{(-0.00148)}{(940s+1)(9s+1)}$	$\frac{(-0.000696)}{(434s+1)(11s+1)}$
g_{21}	$\frac{(0.1636)\,e^{-26s}}{(900s+1)(14s+1)}$	$\frac{(0.09663)\,e^{-26s}}{(520s+1)(12s+1)}$
g_{22}	$\frac{(-0.0255)}{(910s+1)(16s+1)}$	$\frac{(-0.01197)}{(434s+1)(11s+1)}$

Table 6: Transfer Function Models

5.0 Question of Uniqueness

The objective is to ascertain whether relative volatility plays a role independent from holdup in distillation dynamics. Low relative volatility separations typically require large numbers of trays and high internal flow rates. They, therefore, have unusually large holdups. It has never been determined, however, if the large time constants of these columns are an artifact of the large holdup, of the low relative volatility, or of a combination of both.

5.1 Simulation Studies

Simulation studies were made to compare the responses of two columns with the same holdups, but with different relative volatilities (see Table 7).

	high alpha	low alpha
Relative Volatility	1.4	1.15
Total/Feed Tray	42/19	101/45
Top/Bottom Comps.	0.995/0.025	0.995/0.025
Reflux Ratio	4.86	12.79
Tray Holdup (#mol)	24.05	10.00
Total Holdup (#mol)	1010	1010

Table 7 : High and Low Alpha Columns Defined

Simulations were made with feed rate and feed composition disturbances. Both disturbances yielded the same conclusions:

(1) The initial rates of response of the two columns are approximately equal

(2) Return of the high alpha column back to steady state is much quicker

The responses in Figure 19 show a comparison of the two columns when given a square pulse in feed composition of -2%. This study shows no significant difference between the high and low alpha cases suggesting that holdup is the dominating factor in the dynamics of these columns.

5.2 Column Time Constant

The mechanistic basis of this investigation looked at the tray composition time constant from a linearized model.

$$\text{tau tray} = m \,/\, (L + K*V), \tag{8}$$

where m = trayholdup
L = liquid rate
V = vapor rate
K = equilibrium constant

This relationship predicts that the tray composition time constant gets smaller as the relative volatility (or K) gets larger, suggesting the response of the column composition would be quicker for higher K columns. However, this assumes that the other variables remain constant.

In general L, V, and m will all change as the value of K changes. For columns designed at 1.2 times the minimum reflux ratio and the same overhead and bottom compositions, the rates will change as shown below (Table 8).

Relative Volatility	1.4	1.15
L and V (#mol/min)	45	140
m (#mol)	10	30

Table 8 : High / Low Alpha Columns Compared

As the vapor rate increases, the diameter of the column goes up and the holdup on each tray increases. A quick calculation shows that the tray time constant may vary only slightly from low to high alpha columns, and that the column time constant will be predominately dependent on the number of trays and not on the relative volatility of the separation.

The results from both of these investigations (simulation and mechanistic) show that columns which have large holdups and high internal vapor and liquid traffic will behave similarly. It so happens that low relative volatility separations need columns with these characteristics, and, within certain undefined constraints, conclusions drawn about control of the C3 splitter should be applicable for other low relative volatility splitters.

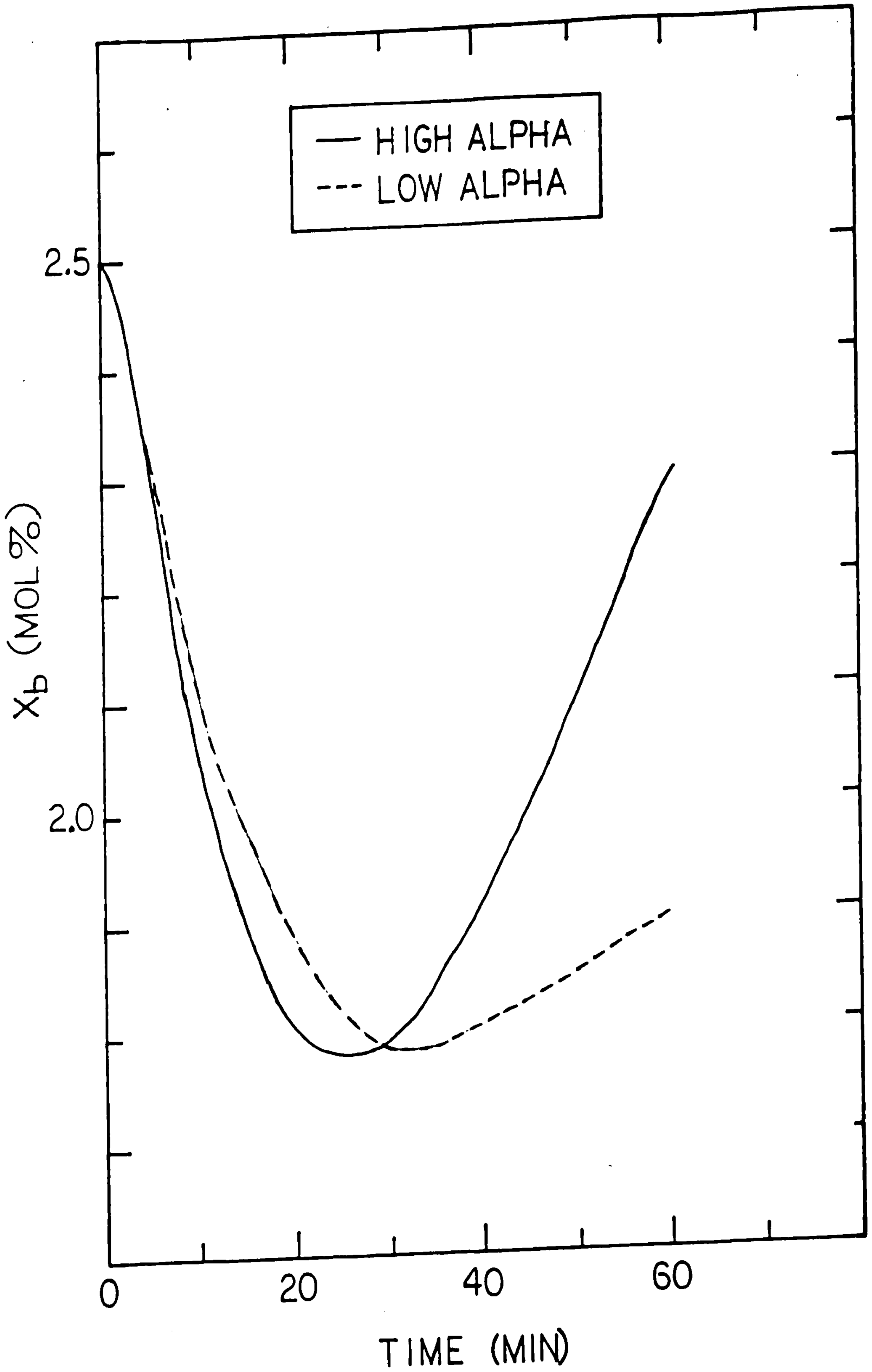


Figure 19: High and Low Alpha Columns Compared

6.0 Control Structure Evaluation

The final and most exciting part of this study involved the synthesis and comparison of the control structures on the dynamic model. This rather exhaustive comparison examined most of the classical single end and dual end composition controllers. In addition, a few less classical structures were tested.

6.1 Steady State Controller Analysis

Henceforth, control structures will follow the nomenclature A/B, where A controls overhead composition and B controls bottom composition. Both A and B could be either distillate flow (D), bottoms flow (B), reflux flow (L), or vapor boilup (V). Using this nomenclature and the following relationships, values for the RGA were found for several control structures. The relationships (assuming constant molar overflow and deviation variables) are:

$$V = L + D \tag{9}$$

$$L = B + V \tag{10}$$

The RGA values calculated are below in Table 9.

Structure	RGA Value
L/V	25.53
D/V	0.08
L/B	0.92

Table 9 : RGA Values for Different Structures

6.2 Tuning Methods

Two basic types of controllers were implemented on the column: level controllers and composition controllers. They are further discussed separately in the following sections.

6.2.1 Level Controller Tuning

The tuning of level controllers is not as critical to the final evaluation of control structures as the tuning of the composition controllers but, a consistent method is required to avoid criticism of the composition controller evaluation. Therefore, the level controllers were tuned as they are in the actual column. This resulted in very tightly controlled levels. The plant settings are found below in Table 10.

Loop	Gain	Resets per Minute
Accumulator Level	2.0	3.03
Bottom Level	1.5	5.06

Table 10 : Level Controller Tunings

6.2.2 Composition Controller Tuning

Initial plans used the transfer functions to derive tuning estimates for the different control structures. In this way, as long as the tuning method was consistent, comparison of control structures with those settings would be consistent. The tuning was performed using the Ziegler-Nichols method and the loops were detuned using the biggest log modulus criterion. When the settings were tested on the model, however, they performed very poorly. There were three possible reasons for these poor responses: (1) poor transfer functions; (2) a poor tuning method; or (3) a poor control structure.

The problem was isolated at the transfer functions. The ultimate gains and periods, found experimentally, were not the same as the ultimate gain and periods found via the transfer functions. This was true even though the time responses of the model and the time responses of the transfer function were very similar for the square pulse input used to identify the column.

There was still a need for a consistent tuning method An experimental approach was used to find the ultimate gains and periods. The method increased the proportional gain until sustained oscillation occurred. The ultimate gain and period were derived from the period and magnitude of these oscillations. This was more computer time consuming but gave us confidence that the tunings were consistent for every control structure. The Ziegler-Nichols settings were then detuned by dividing the gains and multiplying the reset times of both loops by an experimentally determined detuning factor (F). Table 11 gives a summary of the settings and detuning factors used for each composition control structure.

6.3 Level Controllers

Four separate level control schemes were needed to accommodate all of the different composition controllers. They were:

	Accumulator Level	Bottoms Level
(1)	Distillate	Bottoms
(2)	Distillate	Boilup
(3)	Reflux	Bottoms
(4)	Reflux	Boilup

The 32 inch transmitter span was included in the controller action. PI's were used because the actual column level controls are PI and because material balance composition control schemes require tight level controllers.

6.4 Composition Control

The primary evaluation of each control structure was based on how well the composition controllers performed. A consistent method of tuning has already been outlined, now several control structures are evaluated. All preliminary evaluations are shown in Figures 20 through 35, and are briefly discussed in the following sections. Feed rate disturbances are not compared because responses from feed rate changes can be effectively controlled in a feedforward manner. The difficult disturbances to counter are feed composition disturbances, so a +5% feed composition disturbance was used in the preliminary evaluation. In all cases PI controllers are used for composition control.

6.4.1 Single End Controllers

It is sometimes possible to control only one end of a column while leaving the other end open. This eliminates interaction problems and simplifies the control. Unfortunately neither of the single end control structures gave sufficient control of the open end, as was predicted by the rating results (Figures 3-5).

6.4.1.1 Single End Bottom Control

As seen in Figure 20 this structure attempts to hold bottom composition with steam, while leaving the overhead loop open. The system held bottom composition tightly, while the overhead composition drifted unacceptably far away from setpoint (Figure 21).

6.4.1.2 Singe End Overhead Control

Again, the end which was closed was successfully controlled while the end which was open drifted away from setpoint (Figure 23).

Although neither of these structures will be acceptable in final evaluation, they showed that either end can be controlled well and give a standard to compare the responses of two end control structures.

6.4.2 Two End Controllers

An economic incentive to control both ends of the column has already been sited. Single end controllers did not perform well enough to gain the economic advantage of tighter control. An exhaustive review of the performance of classical multiloop single input-single output controllers was made. All evaluations were made using the consistent tuning method and a +5% step in feed composition. These simulations also showed the performance if a constraint was reached with one of the controlled variables or if an analyzer was lost.

6.4.2.1 L/V Structure

The classical energy balance, or L/V structure, (Figure 24) produced stable, yet very sluggish performance. The sluggish response may be a characteristic of these high reflux ratio columns with the L/V structure, and were shown not to be a result of the tuning. As Figure 25 shows, even after 600 minutes neither end is back to setpoint. The RGA for the L/V structure was 25, suggesting interaction between loops.

6.4.2.2 D/V Structure

The RGA for this structure was 0.08. Interestingly, this hints that the reverse pairing of the loops, or the V/D structure, would be superior. In a steady state gain sense this may be true, but dynamically there are big problems controlling the bottom composition with the distillate flow. This was confirmed by simulation.

Nonetheless, the D/V structure (Figure 26) was tested and responses superior to the L/V structure resulted (Figure 27). The overhead was controlled tightly, while the bottom still responds sluggishly.

6.4.2.3 L/B Structure

The RGA analysis predicts that the L/B structure (RGA = 0.92, Figure 28) should perform the best, but the response was still unacceptable (Figure 29). The L/B structure gave tight bottom control, but sluggish overhead control.

6.4.2.4 Reflux Ratio (RR) / Boilup Ratio (BR) Structure

As part of a distillation short course at Lehigh University, F. G. Shinskey gave a demonstration of his 'expert system' for distillation control synthesis. The RR/BR structure is the result of his program (Figure 30).

This structure gave the best response to this point and looked very promising (Figure 31). It gave tight overhead and bottom control with both ends controlling nearly as well as the single end controllers.

6.4.2.5 D/B Structure

The well performing RR/BR structure can be reduced to the D/B structure by assuming tight level control (Figure 32). This significantly reduces the complexity of the structure without impairing the performance. Once again, both overhead and bottoms stay close and return quickly to setpoint (Figure 33). This structure is unconventional, so before application several special characteristics of the D/B structure should be carefully examined. This is done in section 6.5.2.

6.4.2.6 Extensive Variable Control Structure (EVaCS)

The idea of extensive variable control has been proposed. This method uses structural compensators to try to one-way decouple the column. The general form of the controller is shown in Figure 34. The EVaCS gave average response where the overhead and bottoms compositions are both controlled, but only loosely (Figure 35). The response is comparable to the D/V structure response yet less effective than the D/B structure.

6.5 Final Evaluation

Of the eight structures evaluated the best performing were RR/BR and D/B. D/B was the more attractive because it did not require ratio elements and was therefore less sensitive to noisy signals. Its performance was far better than the performance of any other two end controllers, and equaled that of the single end controllers.

For the purpose of actual implementation the D/B structure is also desirable. The current control on the actual column is manual with the operators manipulating distillate to control overhead composition and bottom flow to control bottom composition. The major reason for this is that it is desirable to control levels with large flows (reflux and boilup). One reason is because the orifices for the flow controllers can be considered good to only plus or minus 2%, a tolerance which is nearly the value of the distillate and bottoms flows in these high reflux ratio columns. Current operation has the control structure on manual, so transition to automatic operation would involve closing the loops. The D/B structure also satisfies the criteria set forth by the people at SUN for a desirable structure: (1) the final structure would ideally have levels on large flows; (2) it would be able to be phased in over a period of time (ie. one loop at a time); and (3) it would be explainable in less than 30 minutes. Once again the D/B structure needs special consideration, especially when looking at conditions where a sensor has failed or a valve has saturated.

6.5.1 Additional tests for the D/B Structure

Satisfied that the D/B structure performed best under initial screening, it needed to be tested under more rigorous conditions. The following scenarios were developed to simulate actual operating situations as well as several catastrophic situations. These scenarios are explained figure by figure below.

- Figure 36 : feed composition is dropped 5% (70% to 66.5%)

- Figure 37 : feed rate dropped 20% (15 to 12 #mol/min)
- Figure 38 : feed composition raised 20% (70% to 84%)
- Figure 39 : xb setpoint raised .5% (2.5% to 3.0%)
- Figure 40 : xb setpoint ramped to 5% (2.5% to 5%)
- Figure 41 : xd setpoint raised 0.1% (99.5% to 99.6%)
- Figure 42 : feed quality dropped to 60% (75% to 60%)
- Figure 43 : day / night swings in pressure
  (+20 psi over first 12 hrs., -20 psi over next 12 hrs.)
- Figure 44 : thunderstorm
  (-10 psi over 10 min., regain 10 psi over next 1 hr.)
- Figure 45 : high pressure operation
  (+30 psi over 1 hr., +20% feed comp. @ t=600 min.)
- Figure 46 : low pressure operation
  (-30 psi over 1 hr., -20% feed comp. @ t=600 min.)

These simulations show that the D/B structure handles very large changes in load (Figures 36-38, and 42-44), as well as setpoint changes (Figures 39-41). Figures 45 and 46 demonstrate that this structure is also effective at the extreme operating pressures of the column.

6.5.2 Constraints and Catastrophic Conditions

The actual column at SUN operates at approximately 85% of capacity. The capacity of the column is primarily dictated by the steam valve which saturates before the column floods or any other valve saturates. Likewise, the steam valve in the simulation was spanned to show this characteristic. When the D/B structure was tested for 20% increases in feed (i.e. over capacity) the steam valve saturated and the control failed. For a similar 20% turndown the control structure performed well. This example introduces the question of how to deal with constraint conditions in the column. If the steam valve constraint is reached then a high level override must take over the bottom level. This override should:

(1) recognize the saturated steam valve
(2) override present control and put bottom level on bottom flow while holding steam at present value until level drops to acceptable level.
(3) retain overhead composition on distillate flow while leaving bottom composition uncontrolled

The catastrophic condition which is most likely to upset the column is sensor failure, specifically failure of the on line gas chromatograph. In the case that either analyzer fails, the control must be reduced to the corresponding single end controller.

In general, the D/B scheme was found to perform well under a myriad of extreme conditions. However, the added control does not allow you to exceed the capacity of the column. Constraint and catastrophy overrides must be built into the control system to detect and compensate for these abnormal operating conditions.

Structure	Overhead Loop	Bottom Loop	Detuning Factor
Single End Bottom		K = -1915 K* = -1.17 TAU = 76	2
Single End Overhead	K = -8325 K* = -117 TAU = 50		1
L/V	K = 2475 K* = 2.09 TAU = 192	K = -956 K* = -0.58 TAU = 152	4
D/V	K = -5550 K* = -78.1 TAU = 75	K = -1200 K* = -0.74 TAU = 63	1.5
L/B	K = 4050 K* = 3.41 TAU = 84	K = 338 K* = 18.51 TAU = 80	2
RR / BR	K = -75 K* = N/A TAU = 57	K = 0.40 K* = N/A TAU = 58	1.5
D/B	K = -7500 K* = -106 TAU = 64	K = 360 K* = 19.71 TAU = 69	1.5

* Starred Gains (K*) are dimensionless, unstarred gains (K) are in units given below. Spans : D=213 bph, B=222 bph, L=3550 bph, Stm = 97.9 M-lb/hr distillate comp. = 25% propane, bottom comp. = 100% prope

** Overhead Gains in $\frac{\text{(lb-mol/min)}}{\text{mol\%}}$, Reset Times in Minutes

*** Bottom Gains in $\frac{\text{(lb-mol/min)}}{\text{mol\%}}$ (B structures) or, $\frac{\text{(lb/min)}}{\text{mol\%}}$ (V structures)

Reset Times in Minutes

Table 11. Composition Controller Tuning Summary

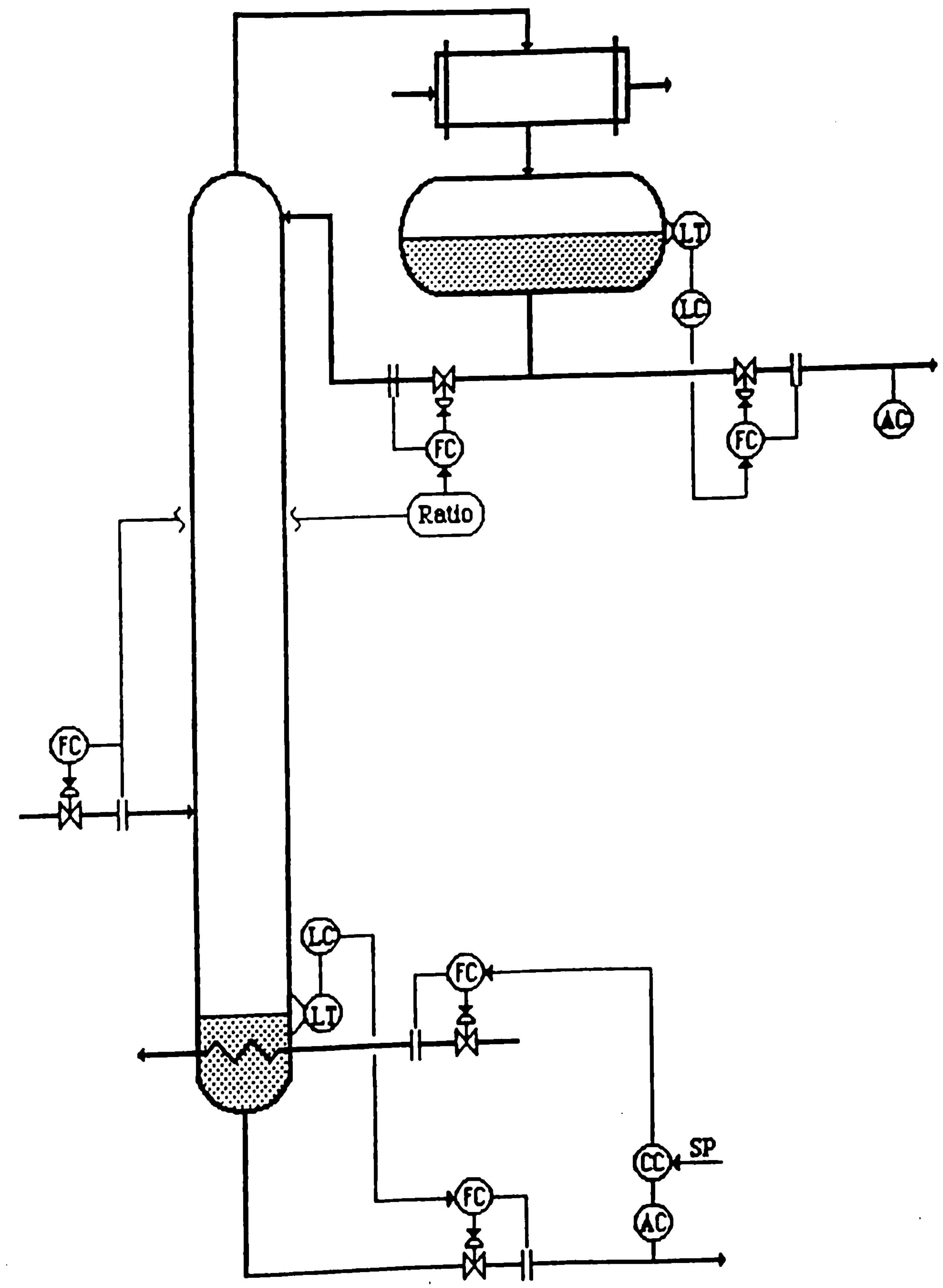


Figure 20: Single End Bottom Structure

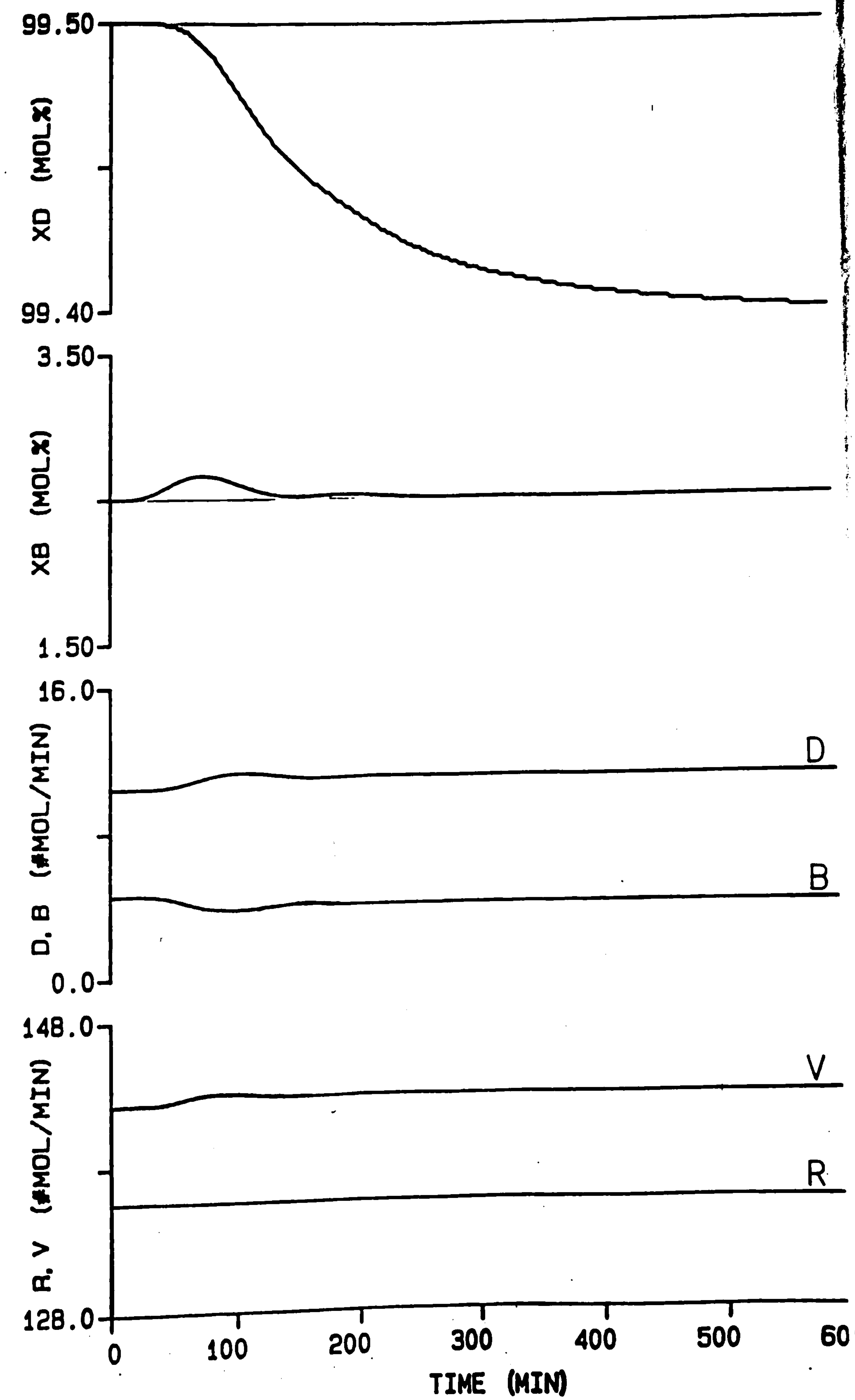


Figure 21: Response of Single End Bottom Structure

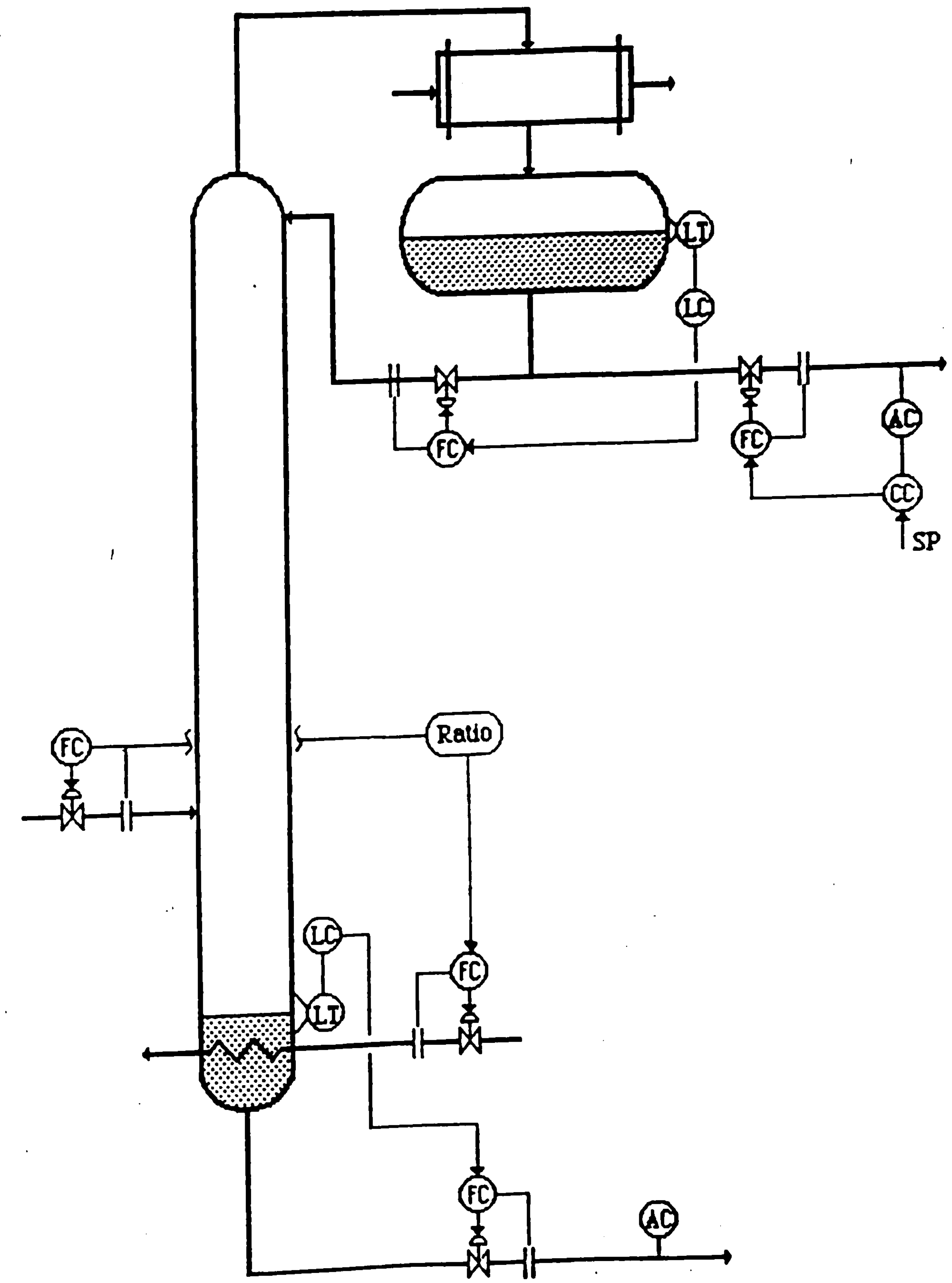


Figure 22: Single End Overhead Structure

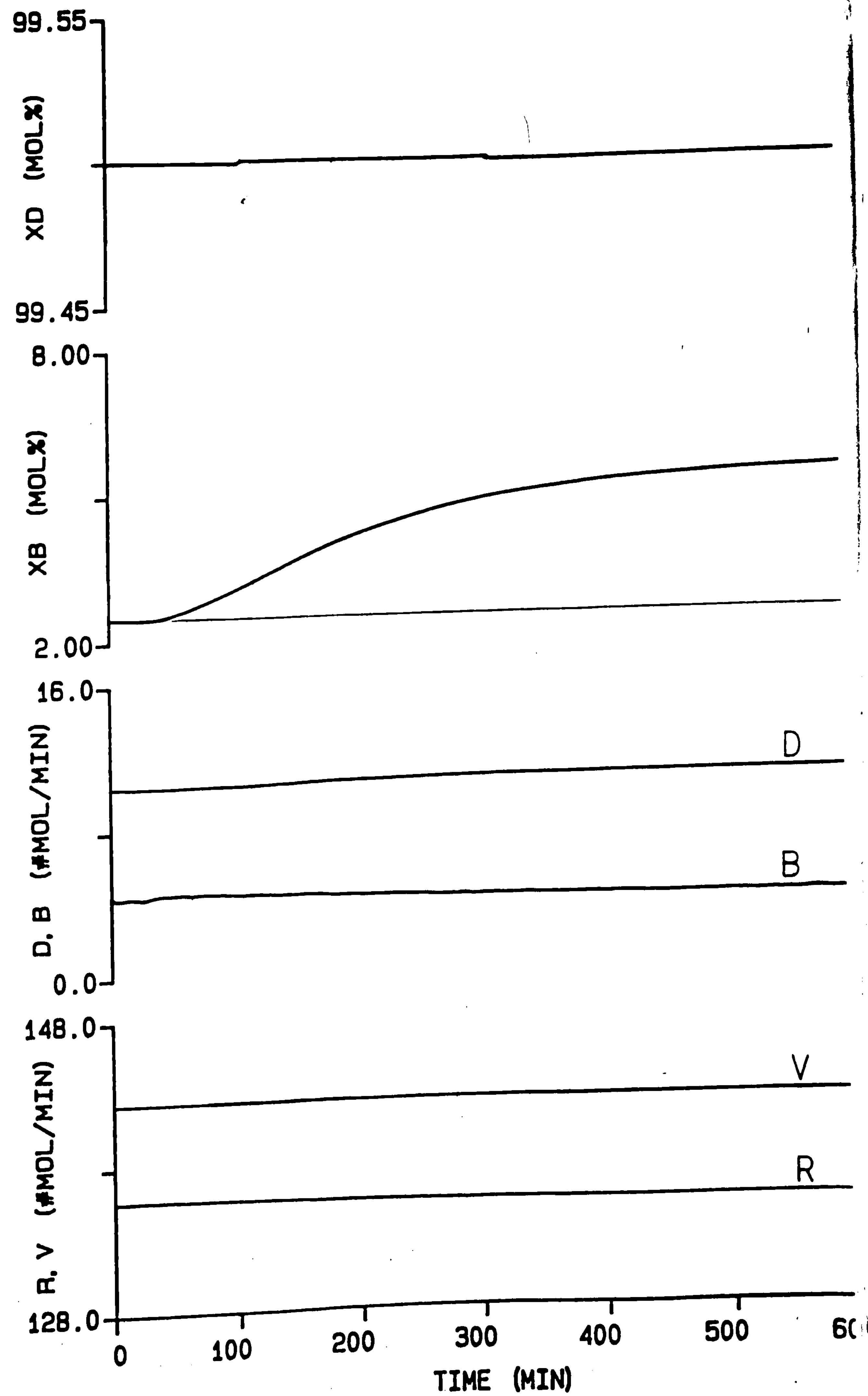


Figure 23: Response of Single End Overhead Structure

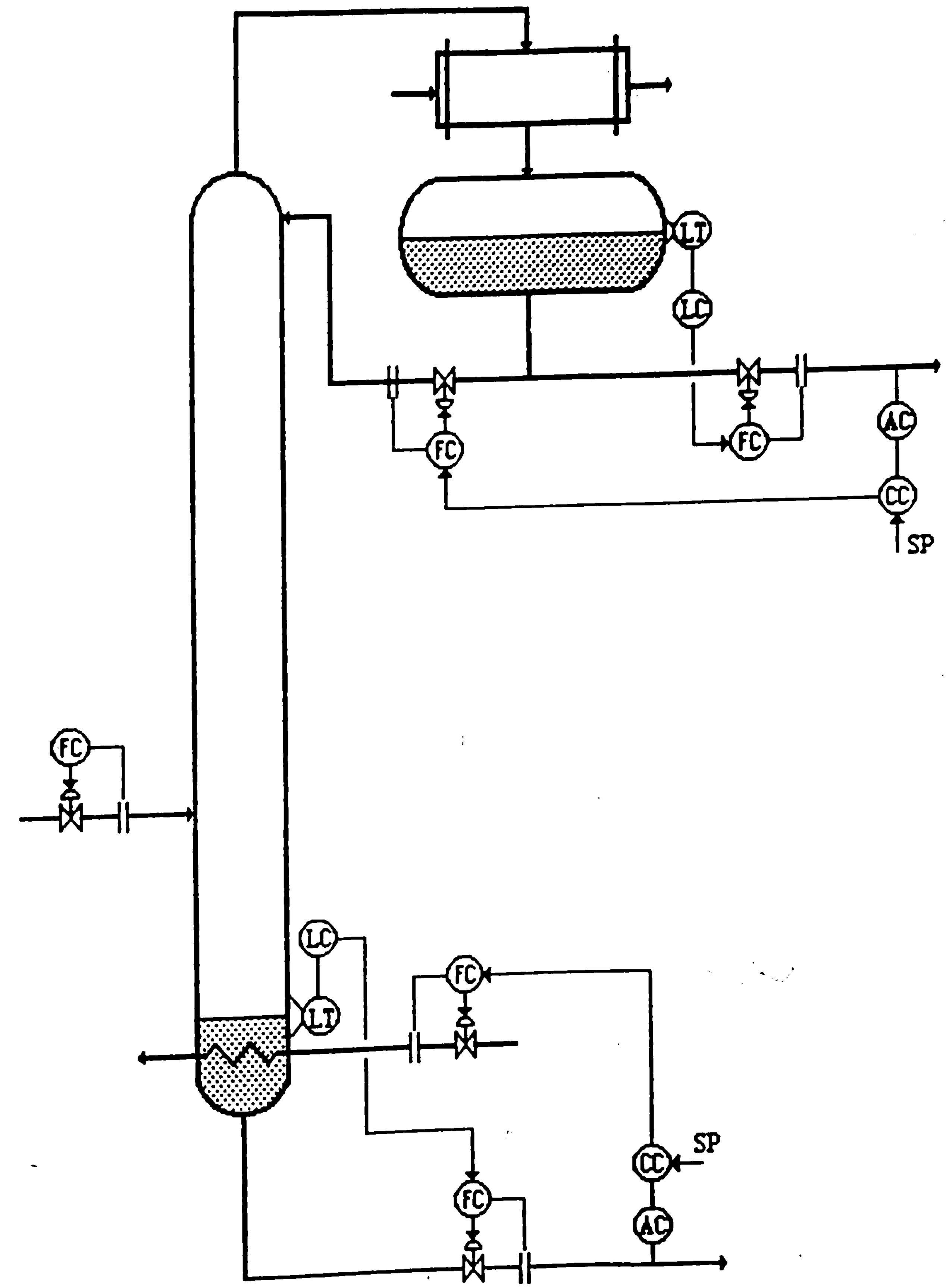


Figure 24: L/V Structure

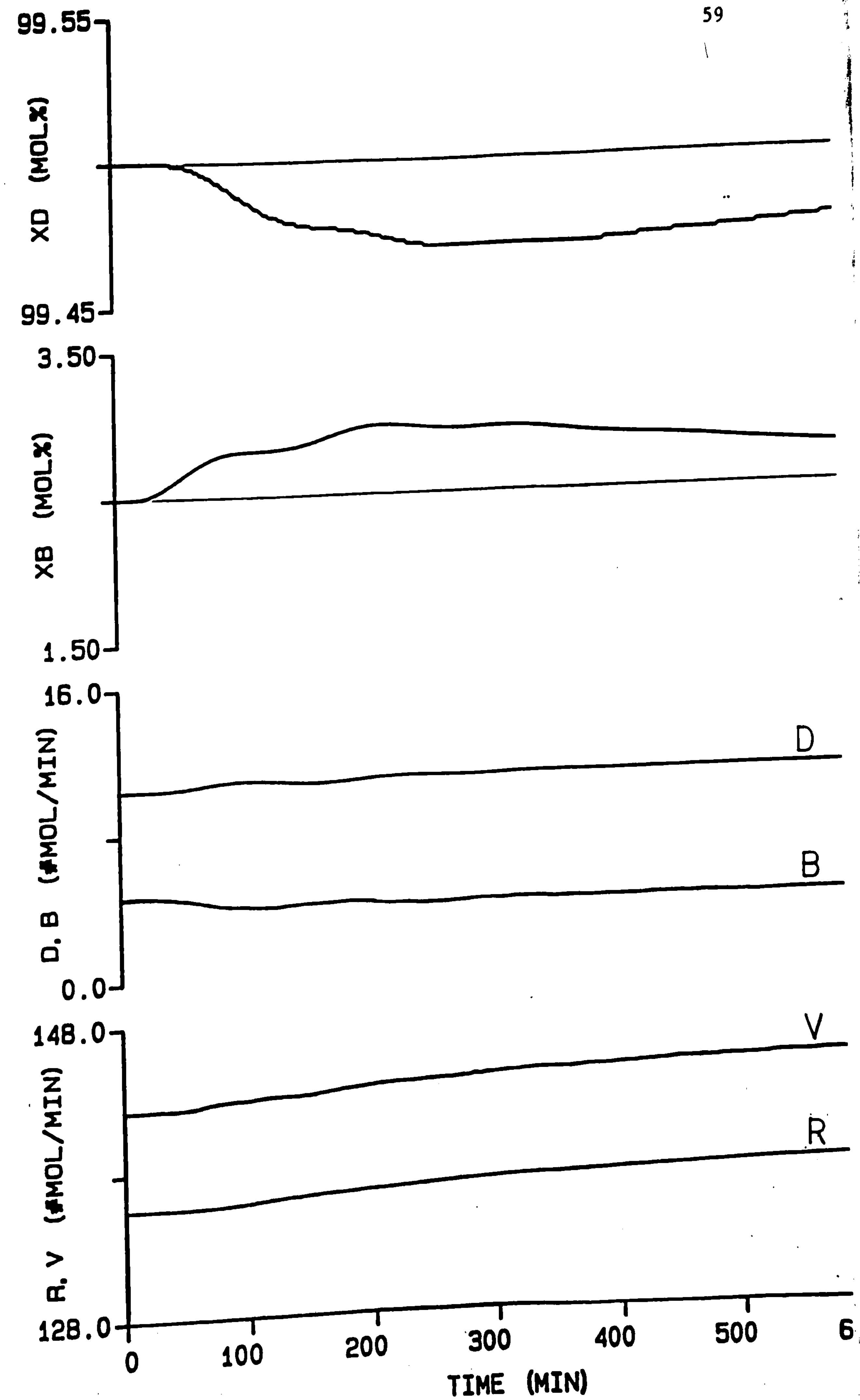


Figure 25: Response of L/V Structure

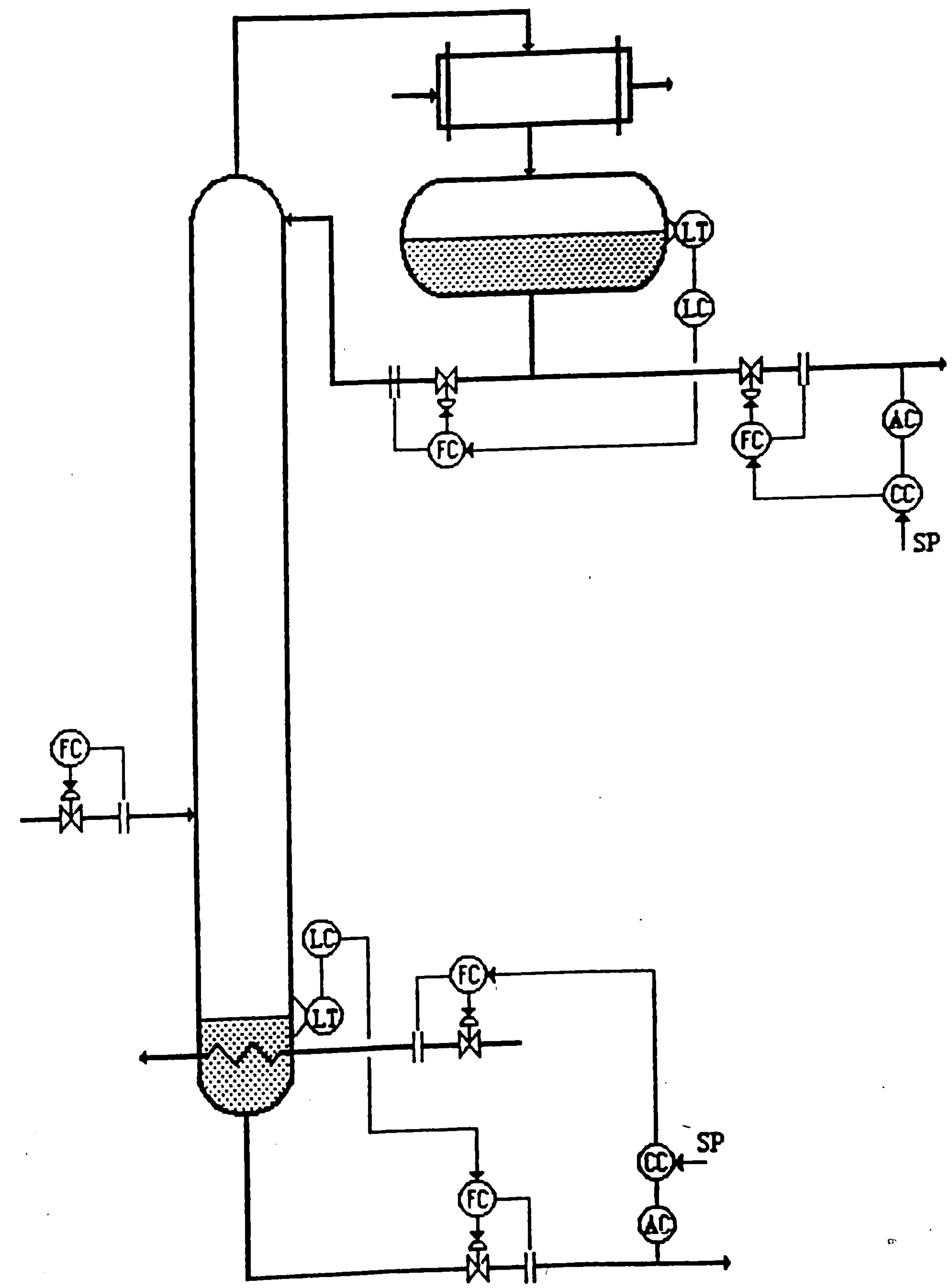


Figure 26: D/V Structure

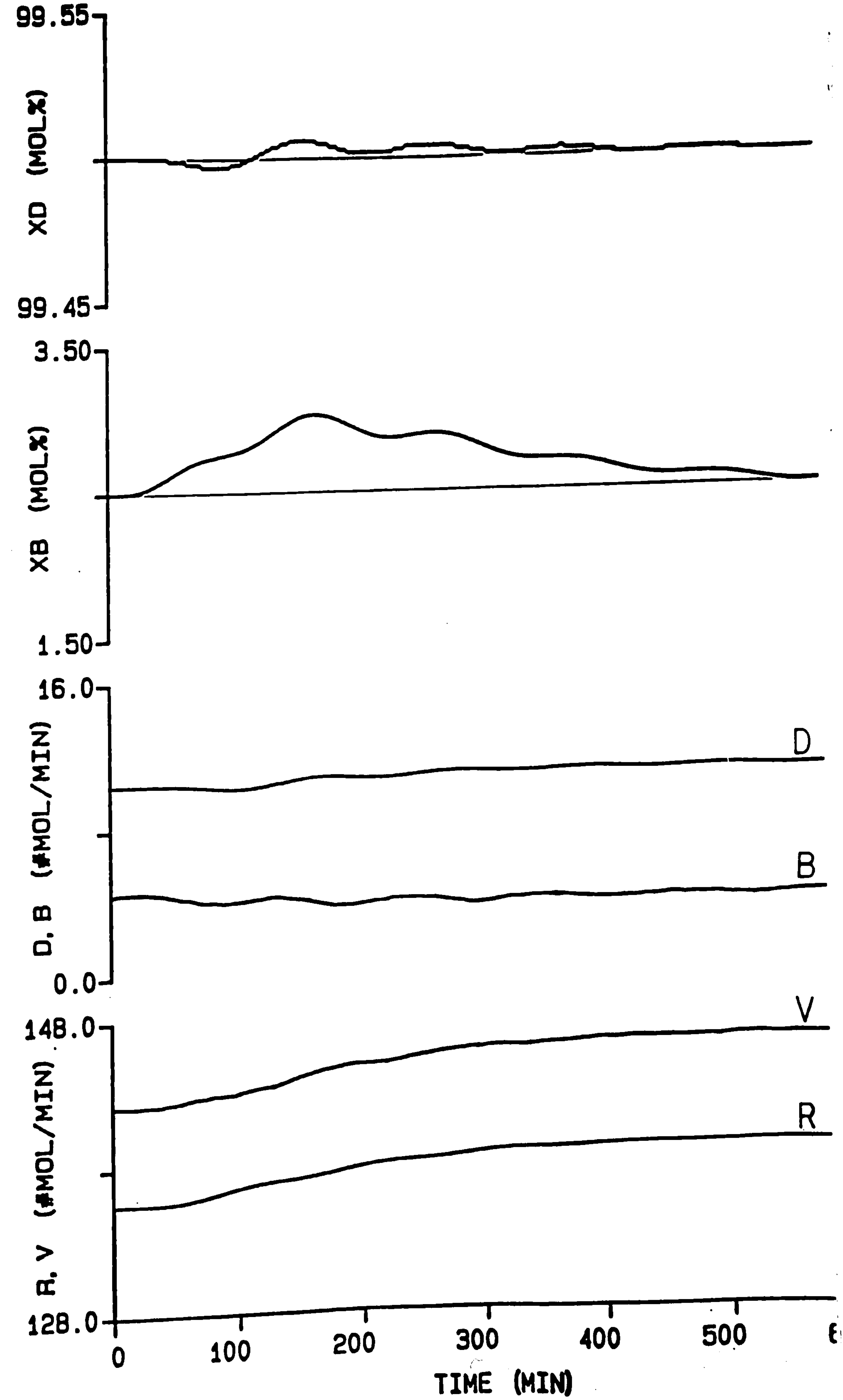


Figure 27: Response of D/V Structure

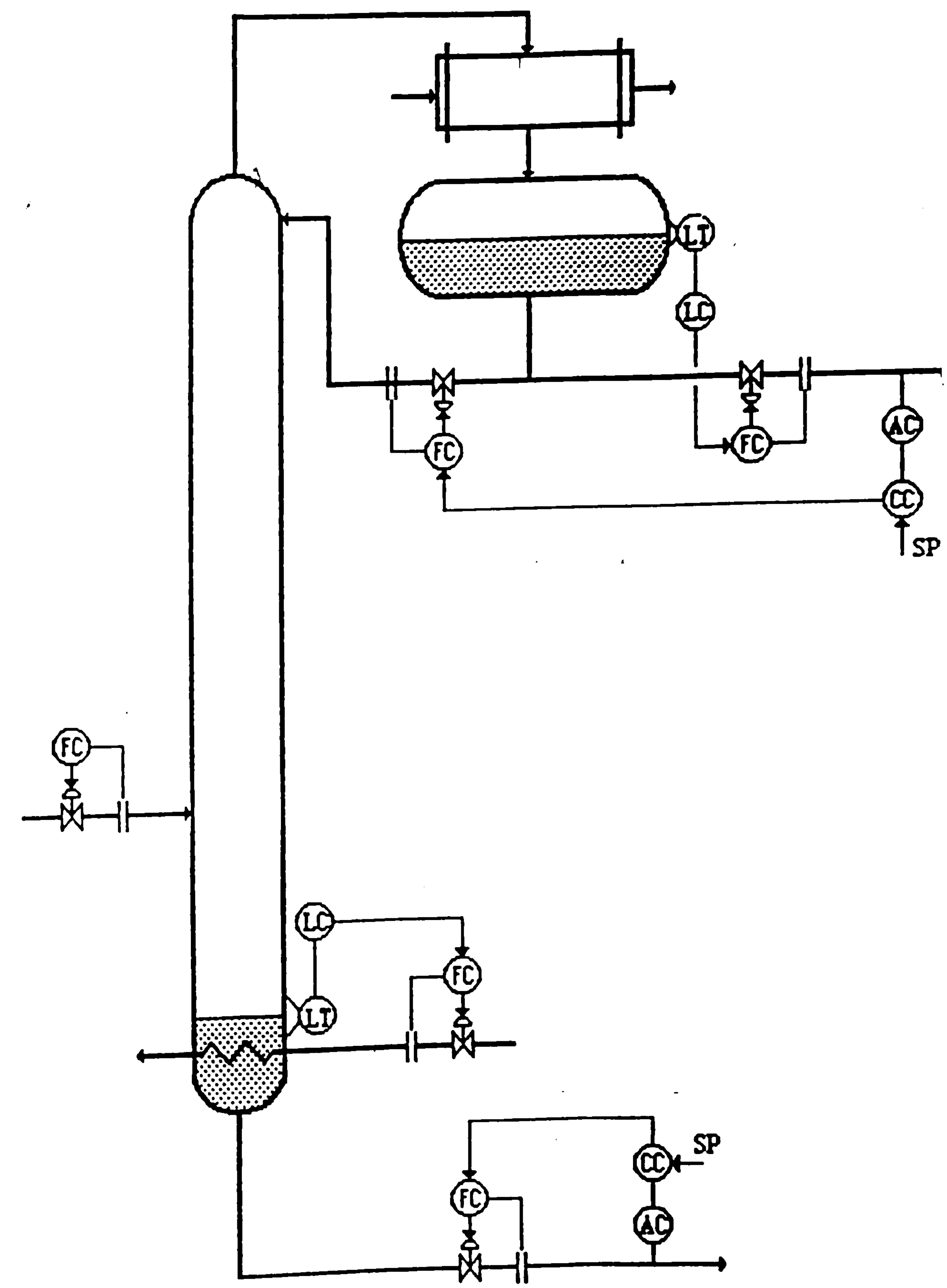


Figure 28: L/B Structure

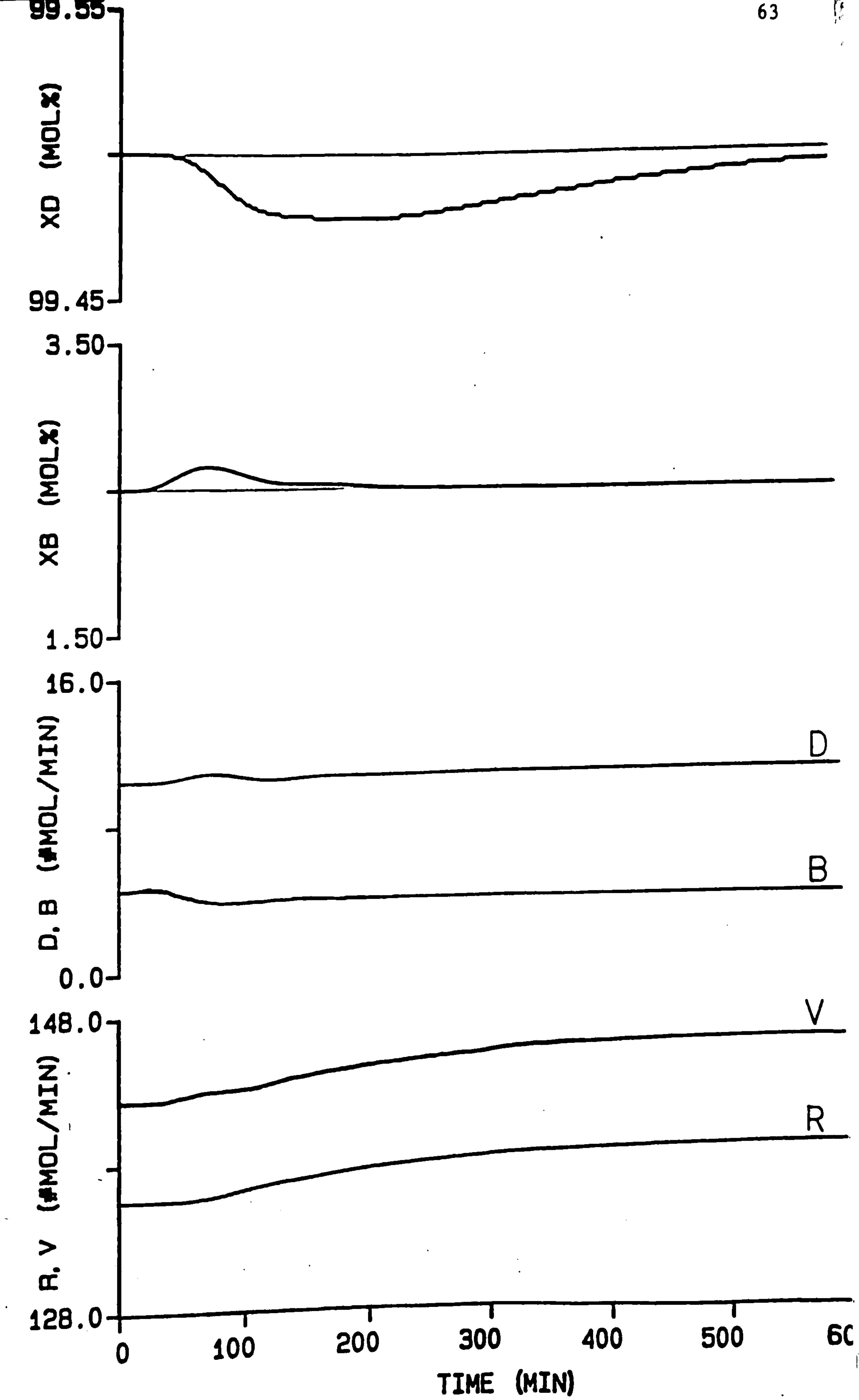


Figure 29: Response of L/B Structure

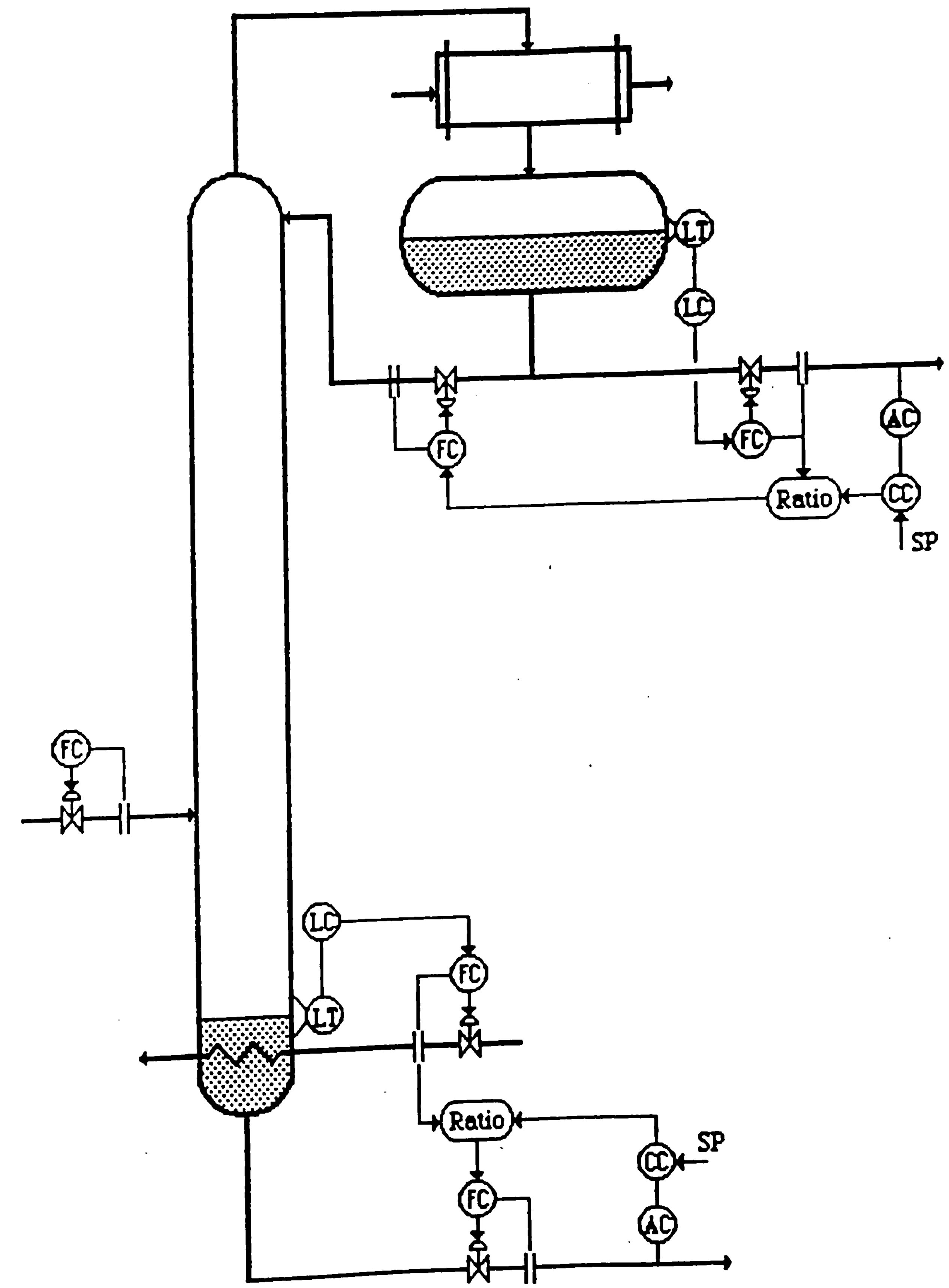


Figure 30: Reflux Ratio / Boilup Ratio Structure

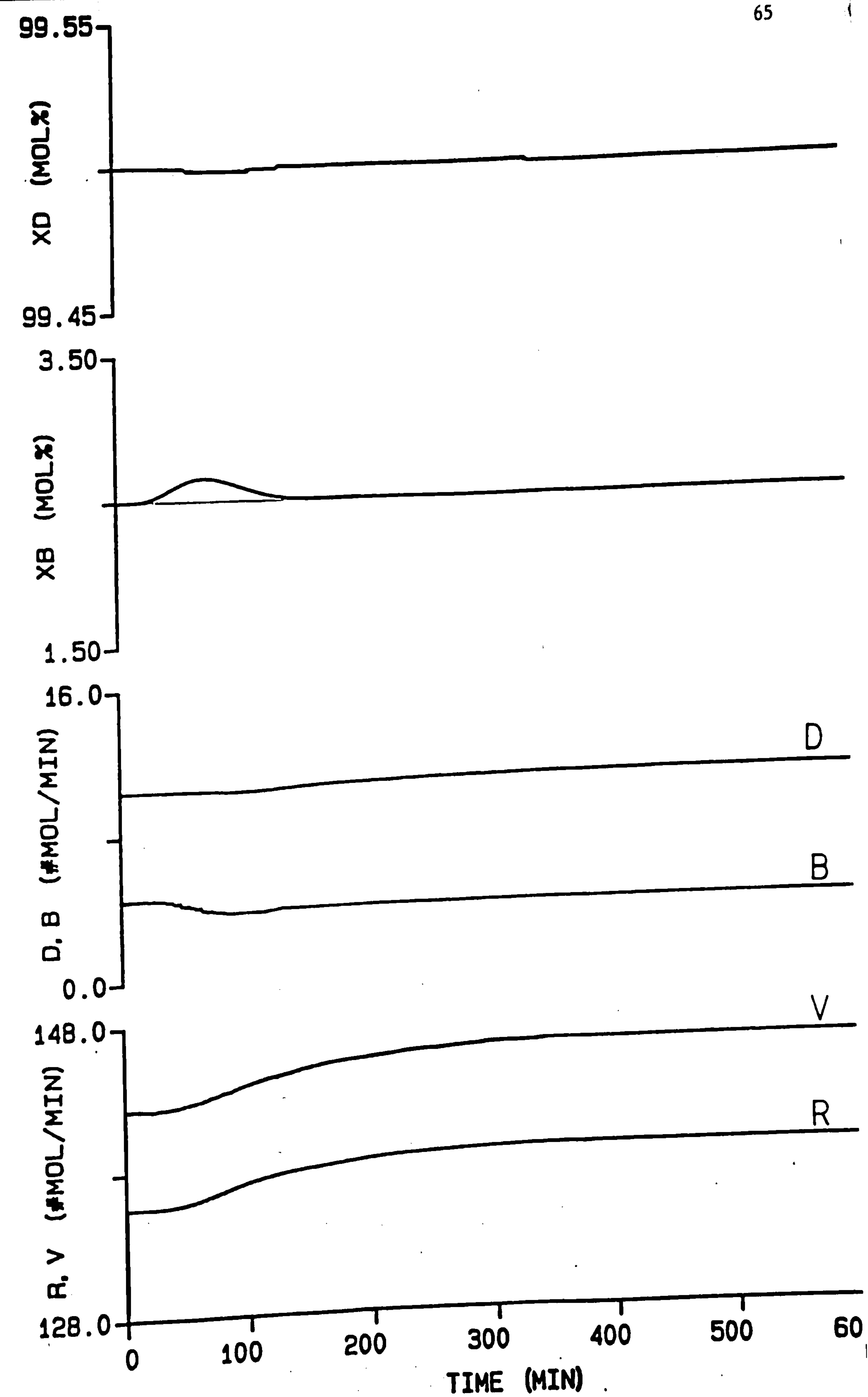


Figure 31: Response of RR/BR Structure

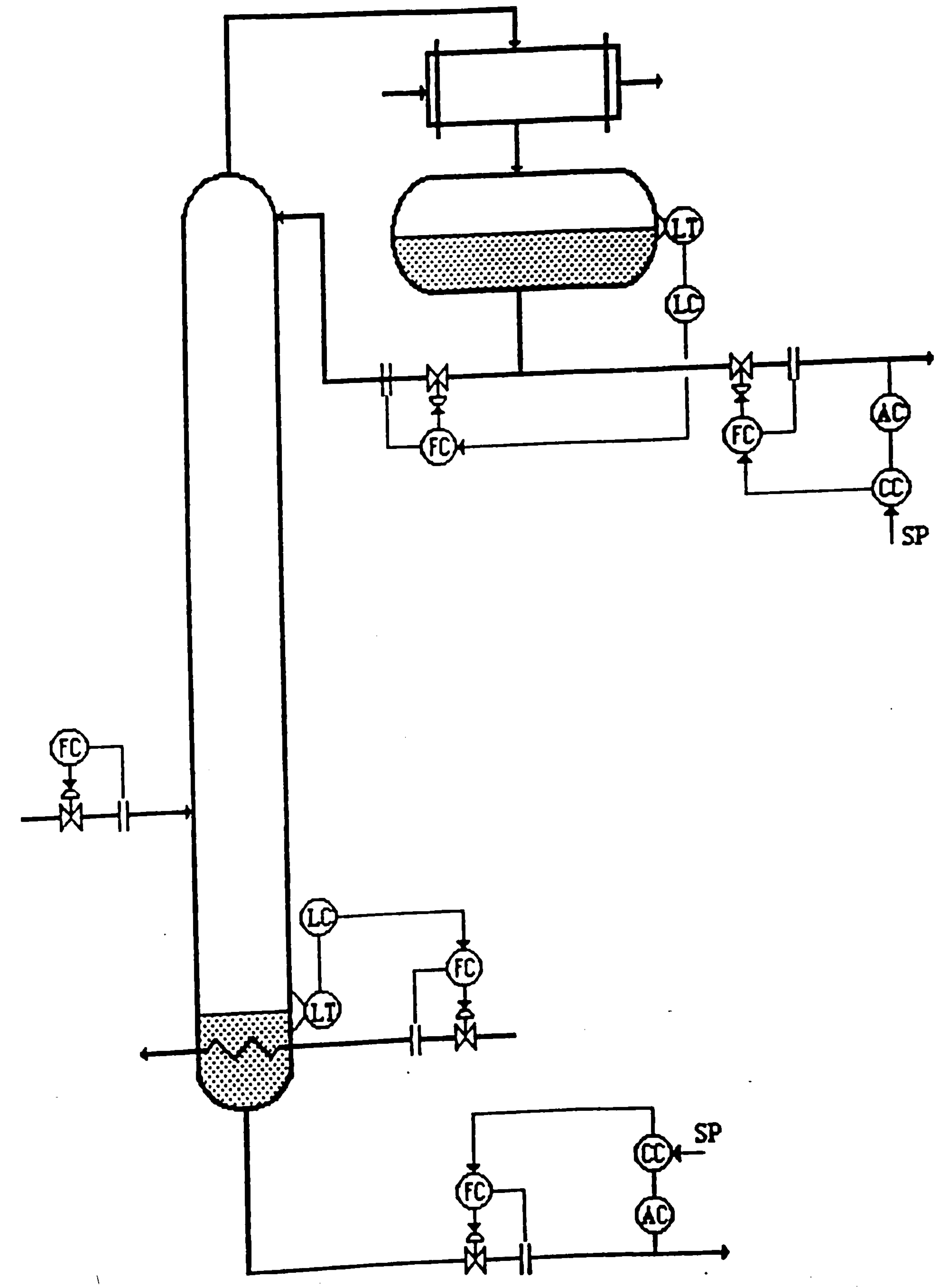


Figure 32: D/B Structure

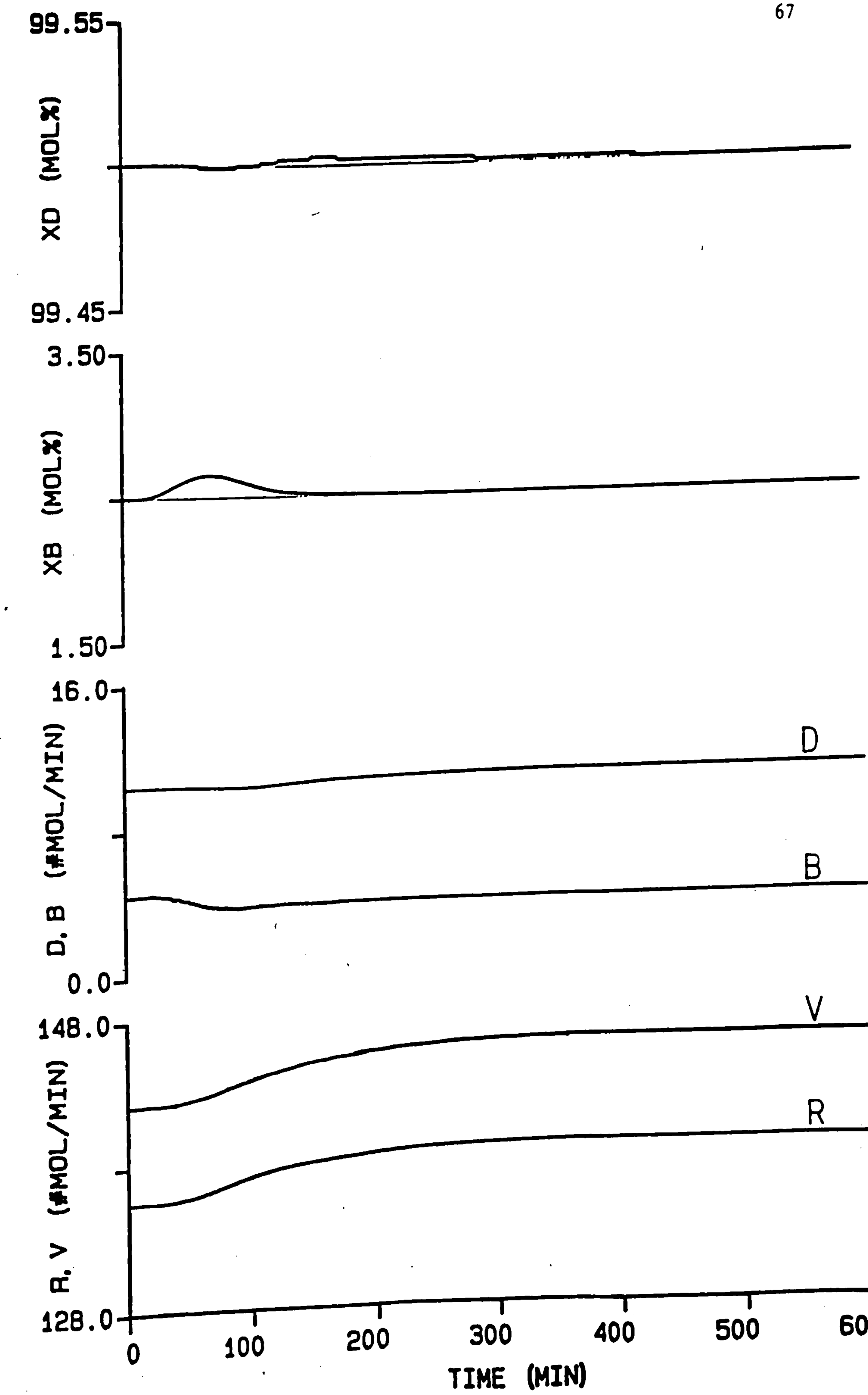


Figure 33: Response of D/B Structure

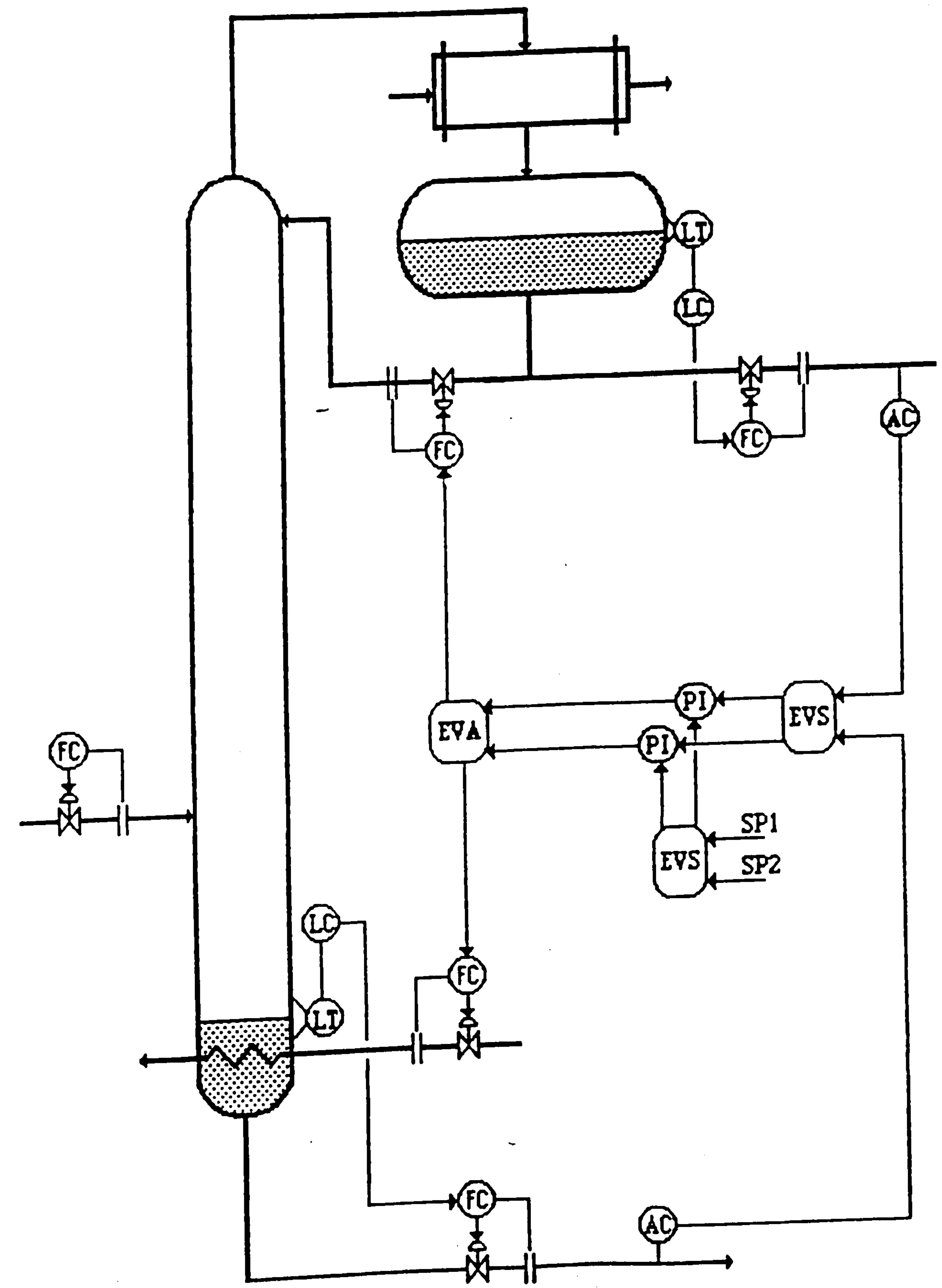


Figure 34: EVaCS Structure

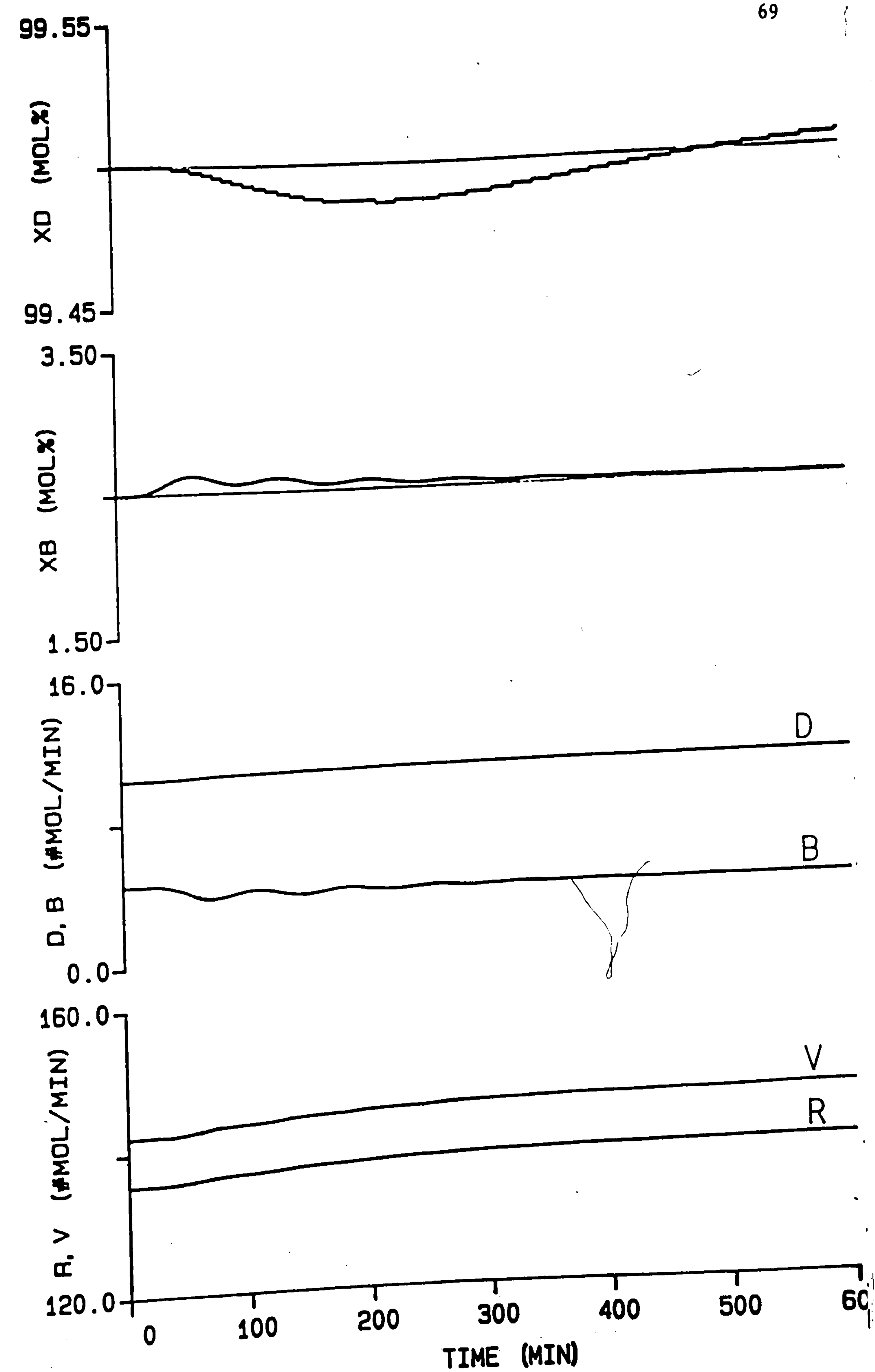


Figure 35: Response of EVaCS Structure

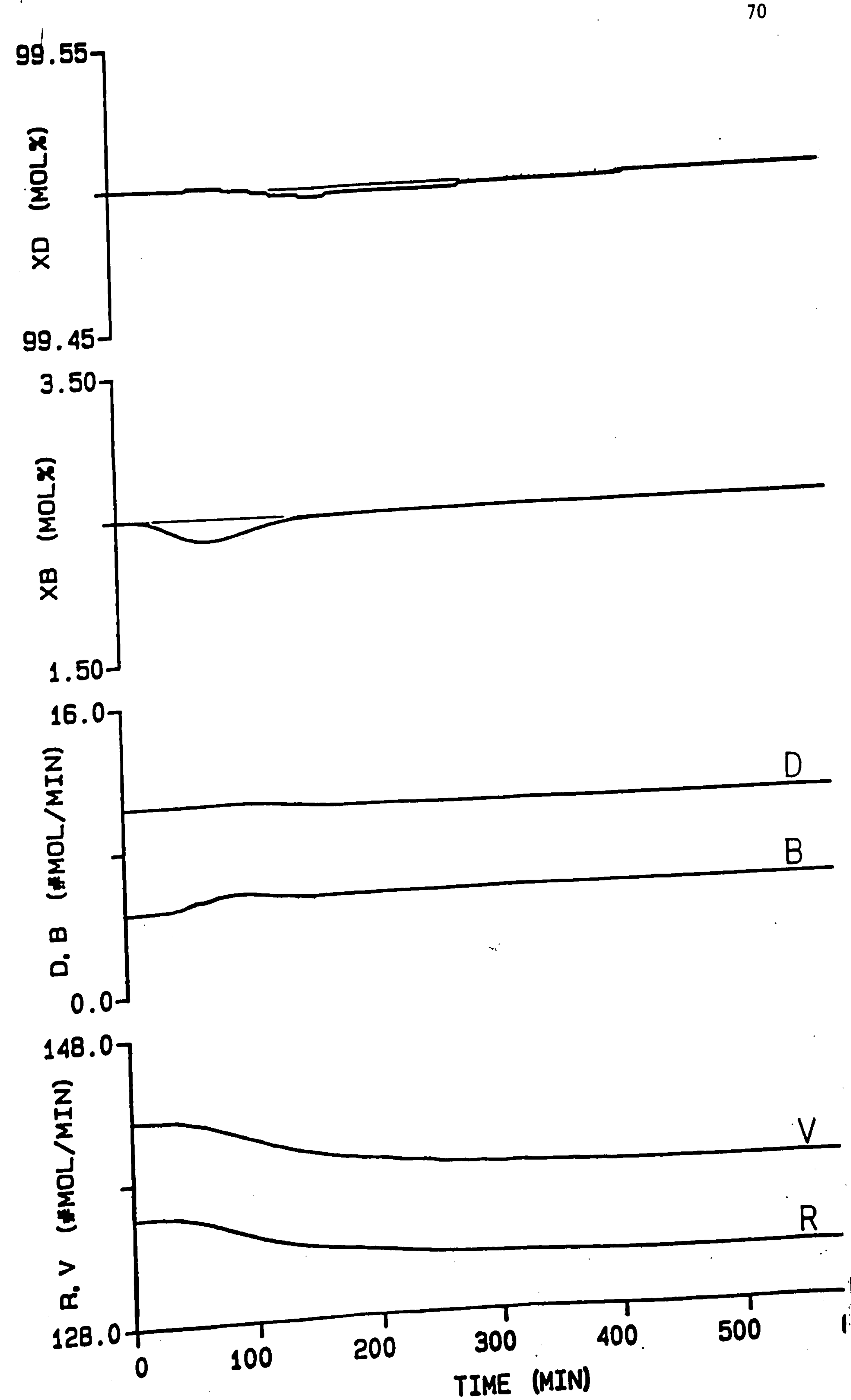


Figure 36: D/B Structure, 5% drop in Feed Composition

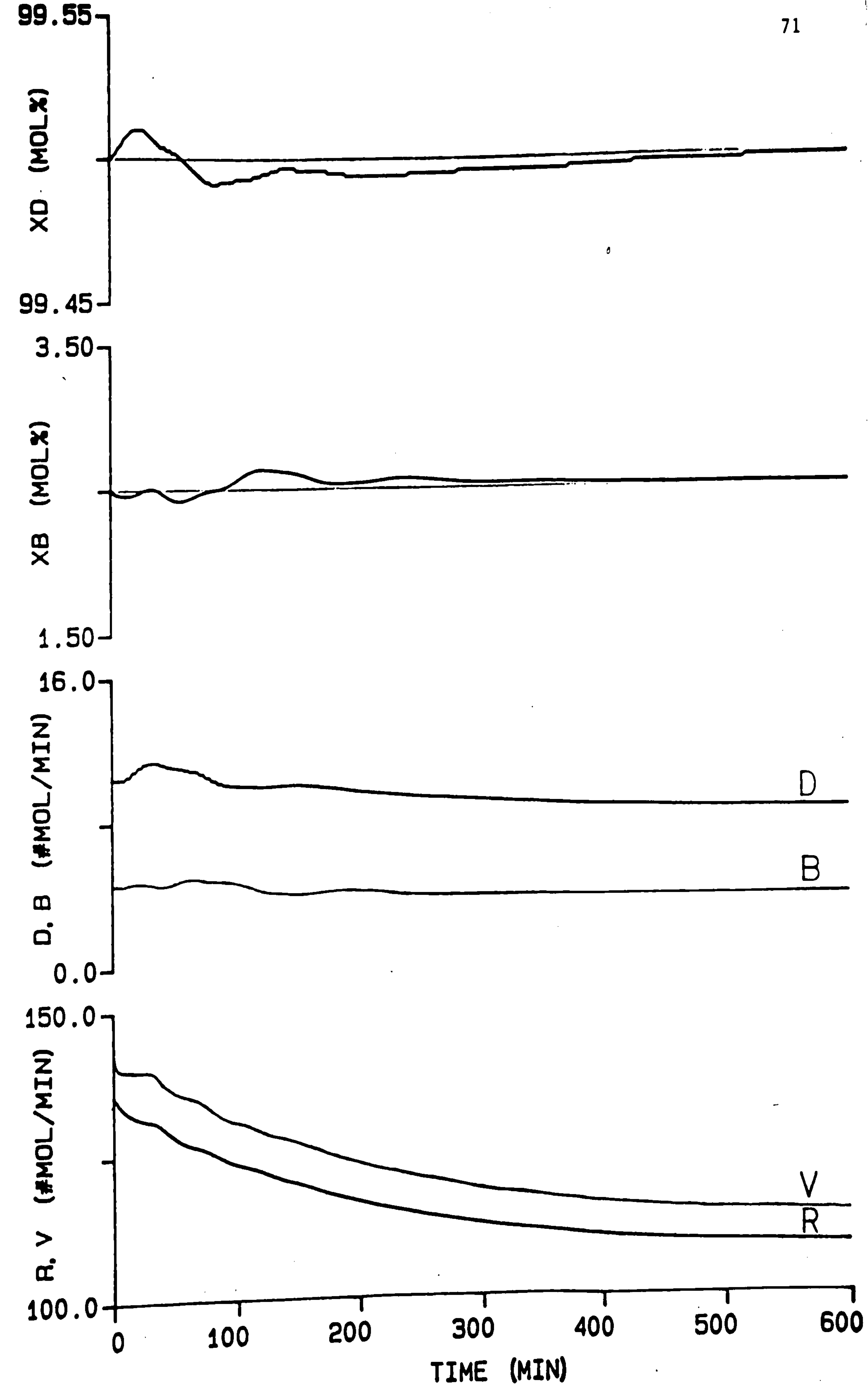


Figure 37: D/B Structure, 20% drop in Feed Rate

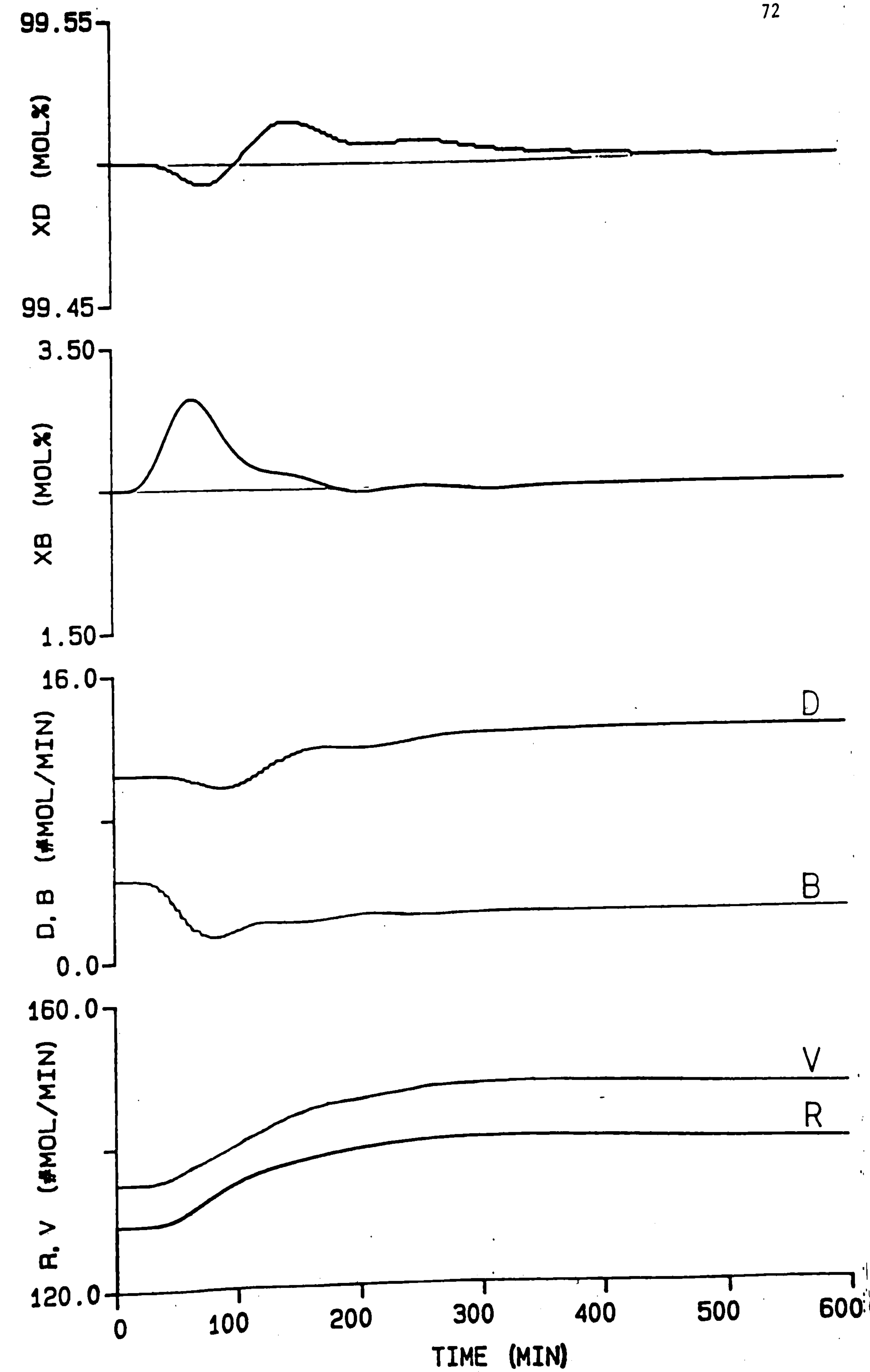


Figure 38: D/B Structure, 20% increase in Feed Composition

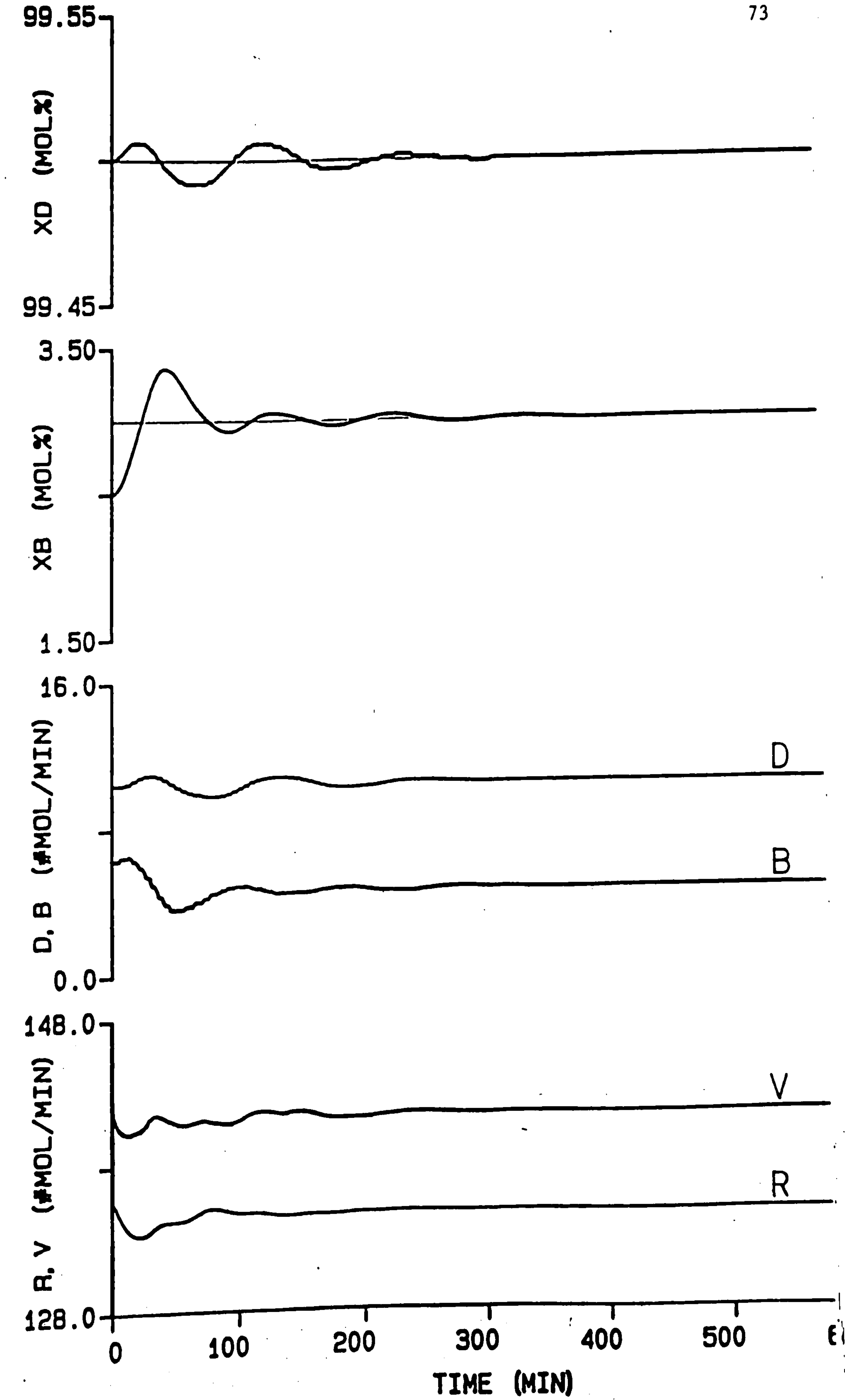


Figure 39: D/B Structure, Bottom Setpoint to 3%

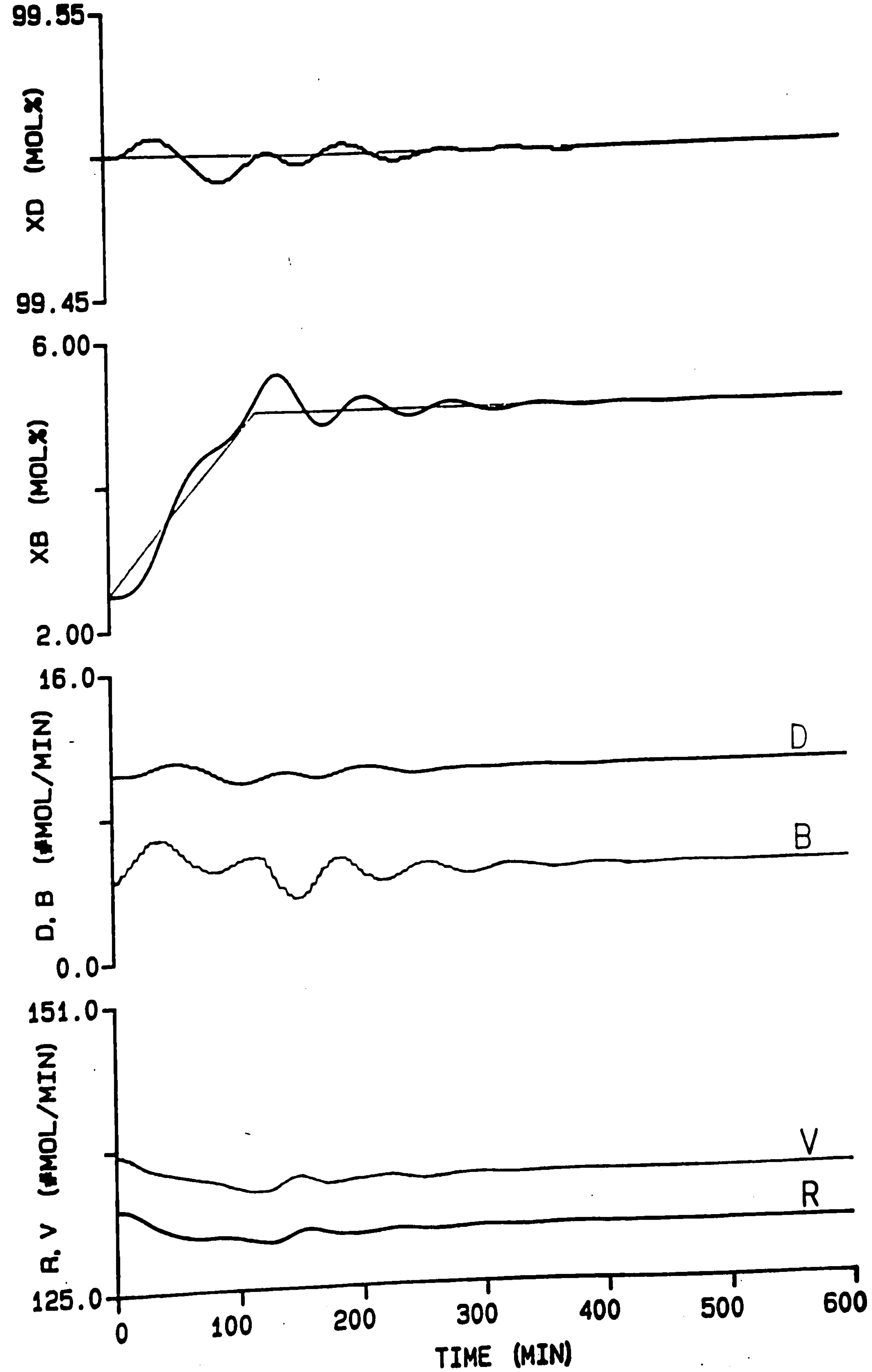


Figure 40: D/B Structure, Bottom Setpoint ramped to 5%

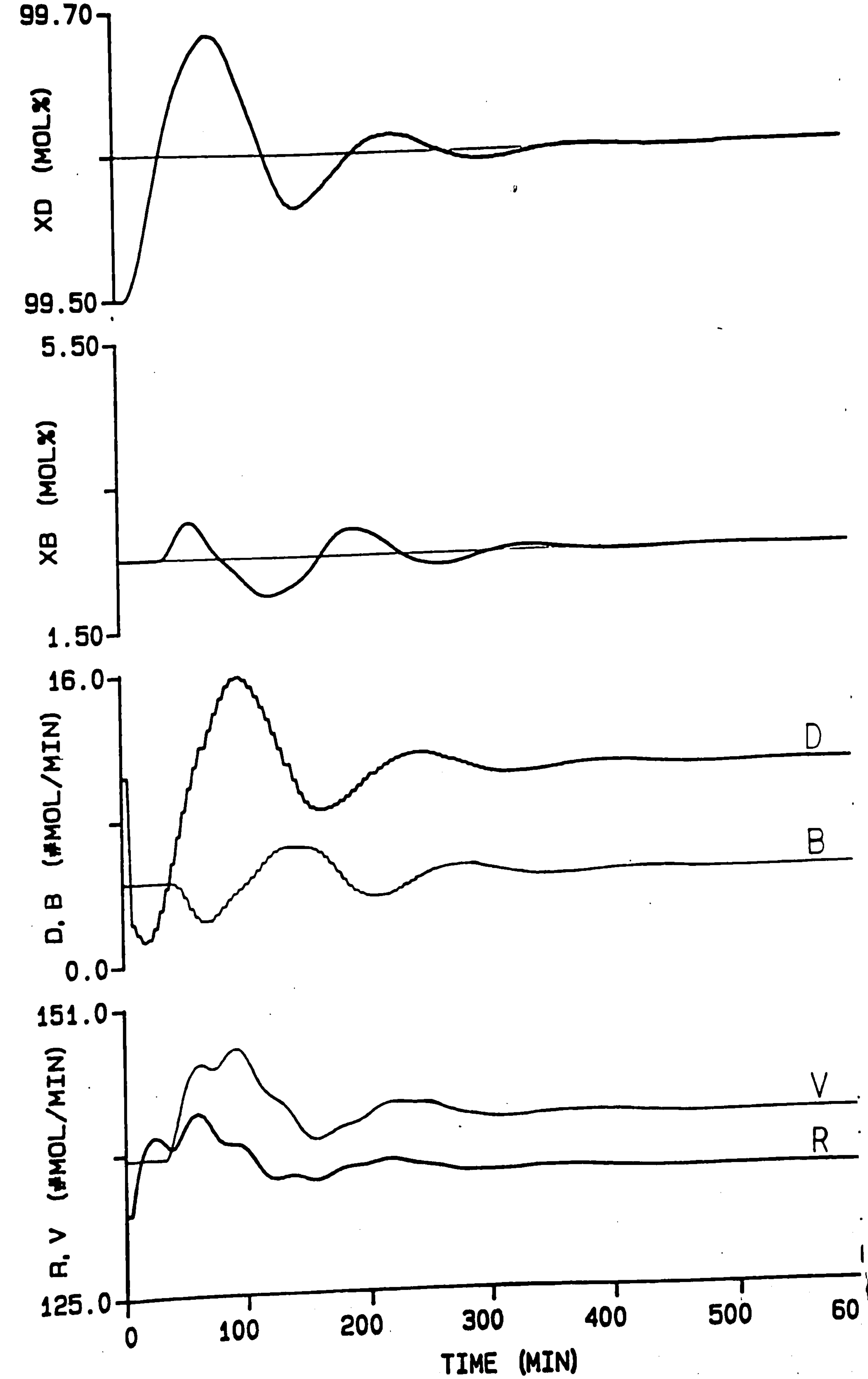


Figure 41: D/B Structure, Overhead Setpoint to 99.6%

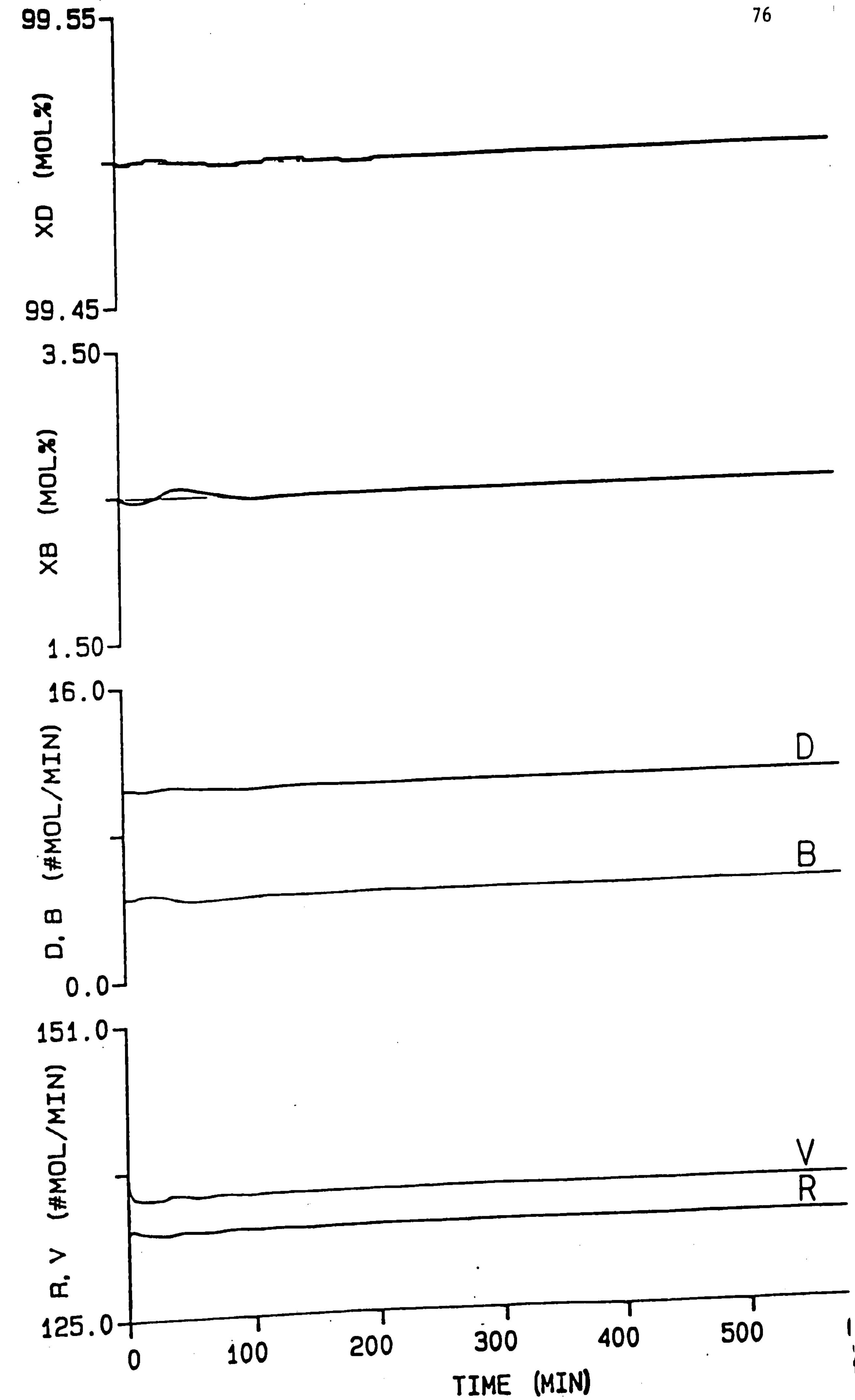


Figure 42: D/B Structure, Feed Quality dropped to 60%

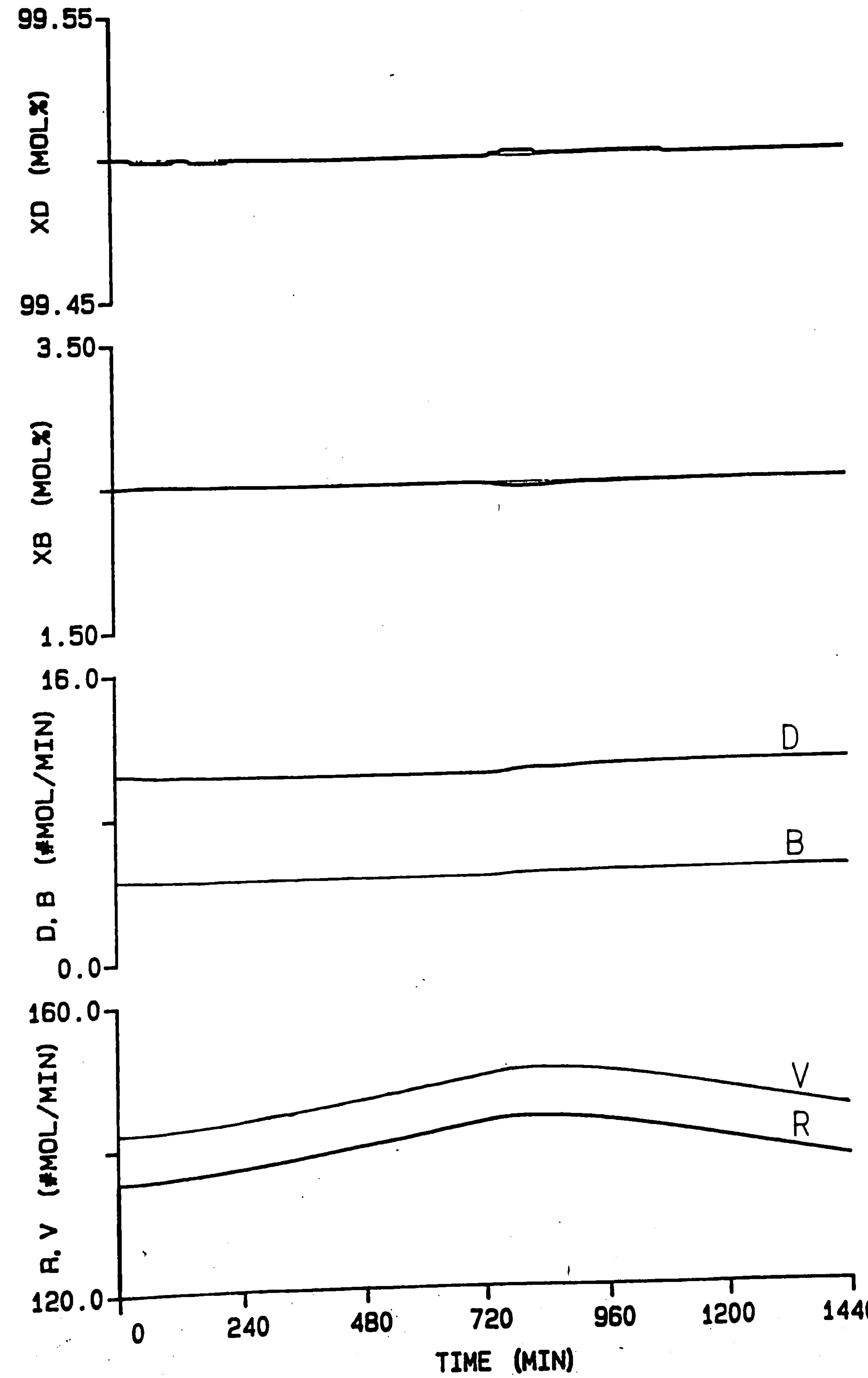


Figure 43: D/B Structure, Day/Night Pressure Swings

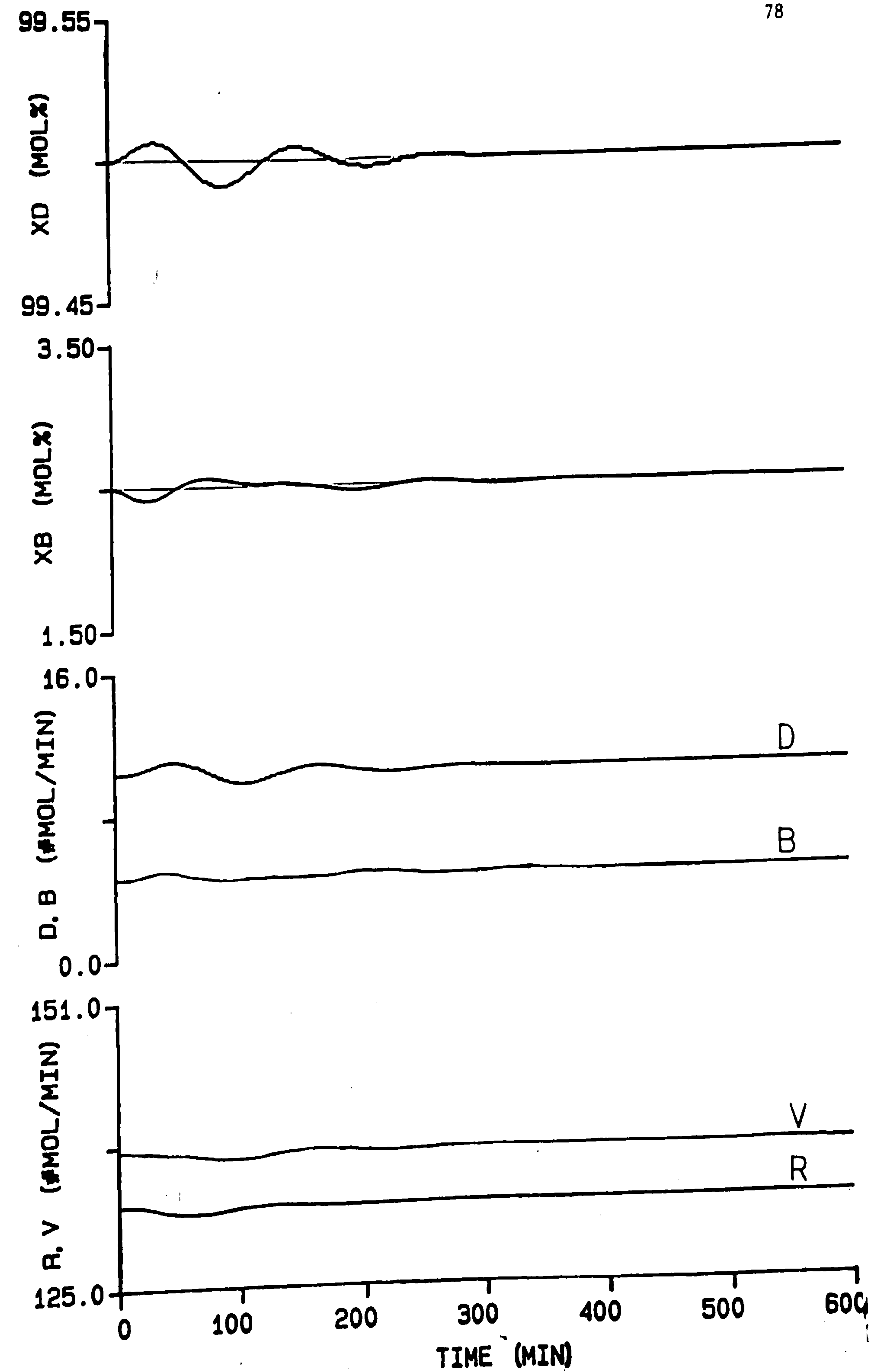


Figure 44: D/B Structure, Thunderstorm

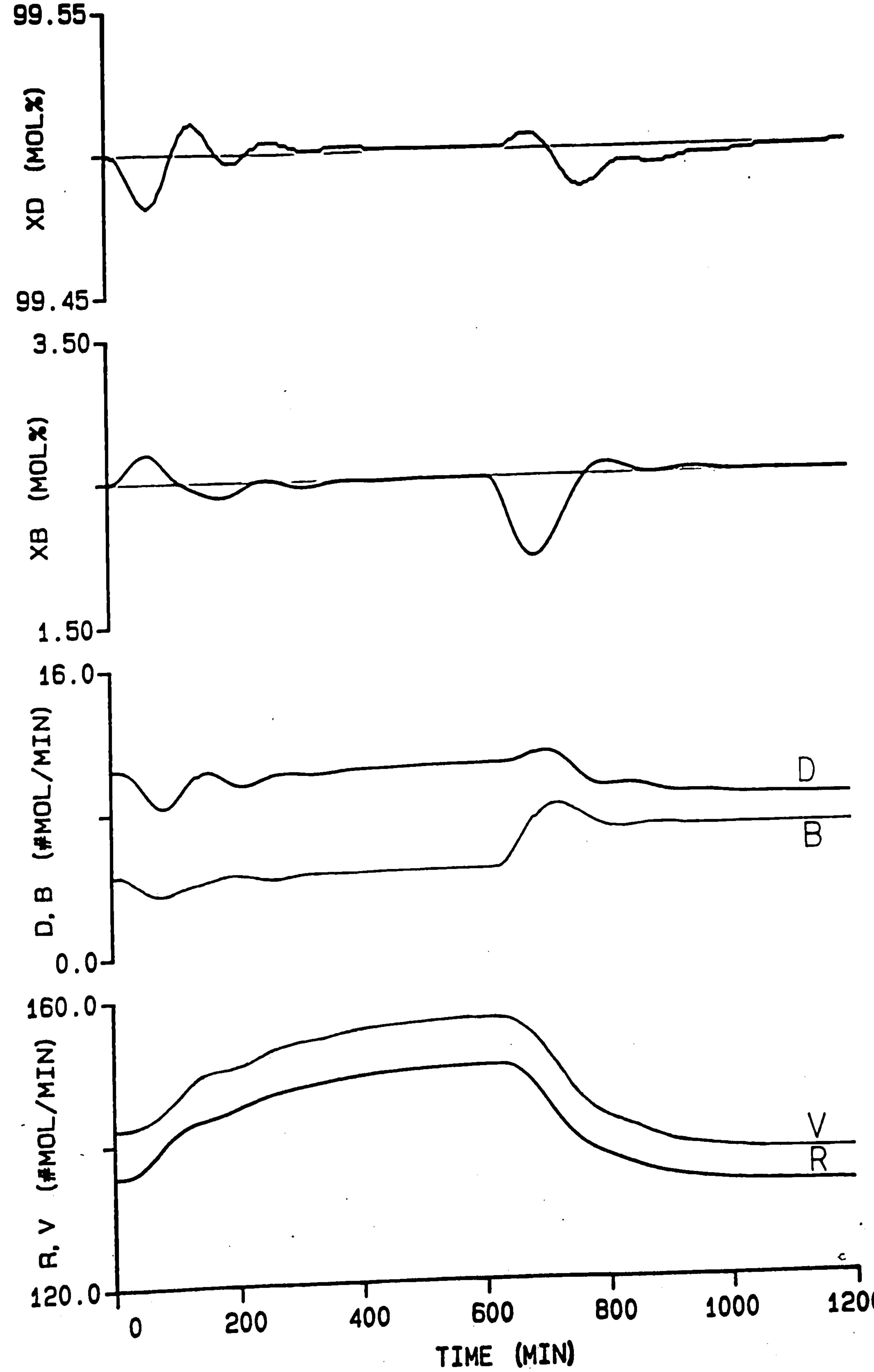


Figure 45: D/B Structure, High Pressure Operation

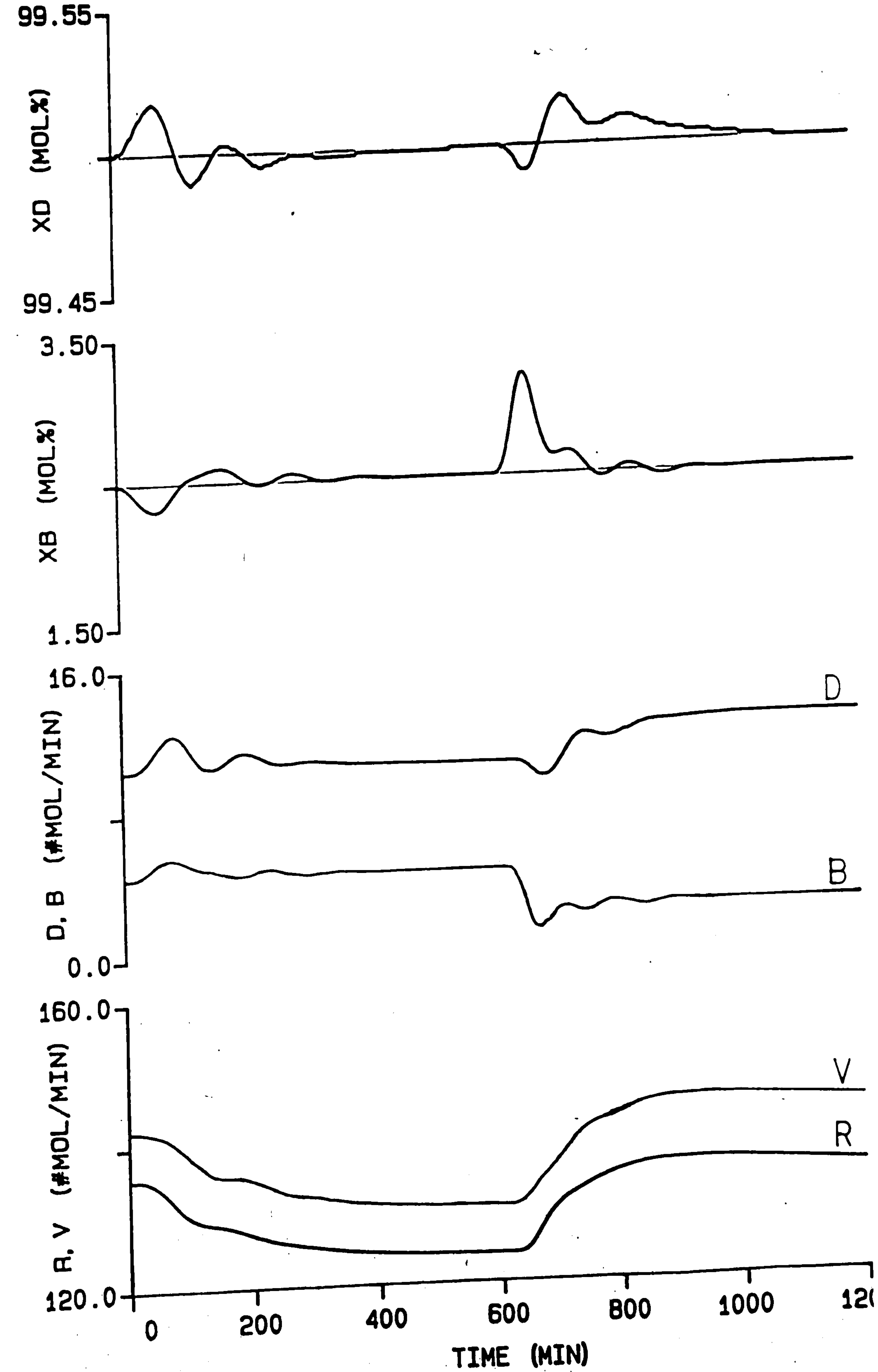


Figure 46: D/B Structure, Low Pressure Operation

7.0 Conclusions and Future Work

In preliminary evaluation the D/B structure performed best and was also a simply implementable structure. Minimal resistance to the structure should be encountered at the refinery because the D/B structure is similar to the present manual mode of operation. When tested under normal and extreme conditions the D/B structure performed well and is therefore recommended to be implemented with consideration given to saturated valve and analyzer failure conditions discussed in section 6.5.2.

Several questions have been left unanswered by this thesis, however. The first question asks how reliable transfer function models can be obtained for low relative volatility, high purity columns. This is not a new question, but an extremely important one. The problem was successfully avoided by finding the ultimate gains and periods experimentally and therefore bypassing the need for transfer functions in tuning. The transfer functions would, however, be needed to do frequency domain controller analysis. The method which I used is therefore a short cut and not a solution.

The second unanswered question is how to estimate the composition at one end of the column given the other end's composition and available process variables (i.e. pressure, reflux, feed, distillate, and bottom flows). The estimation could be used to back up the gas chromatograph and, ultimately, to control from if the analyzer fails. The estimation should be possible because the column is nearly ideal with constant molar overflow and low relative volatility.